AD-780 301

PHAS2O, A PROGRAM FOR SIMULTANEOUS MULTIPLE REGRESSION OF A MATHEMATICAL MODEL TO THERMOCHEMICAL DATA

GEOLOGICAL SURVEY

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PHAS20 performs simultaneous multiple regression of a mathematical model for the functional relations among the thermodynamic quantities to experimental data for a group of chemically related species. The thermodynamic quantities included are heat capacity, entropy, enthalpy, free energy, equilibrium constant, electrochemical potential, and relative heat content. Without further adjustment, PHAS20 will fit the model to 70 sets of data containing a total of 1200 observations on 20 species. The data may include any and all of the following types of observations: 1) for individual species; heat capacity, third law entropy, enthalpy of formation from oxides and elements, free energy of formation from oxides and elements, and relative heat content data such as are obtained from drop calorimetry; 2) for reactions; heat capacity change, entropy change, enthalpy change, enthalpy change of a transition (e.g., heat of fusion, heat of vaporization, etc.), free energy change, equilibrium constant, and electrochemical potential.

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COMPUTER CONTRIBUTION

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PHAS20, A Program for Simultaneous Multiple Regression of a Mathematical Model to Thermochemical Data

by

John L. Haas, Jr.

U.S. Geological Survey

Washington, D. C.

1974

Program Number:	G466
Equipment:	IBM 360/65
Operating System:	IBM System 360
Language:	FORTRAN IV

12

CONTENTS

ABSTRACT

PHAS20 performs simultaneous multiple regression of a mathematical model for the functional relations among thermodynamic quantities to experimental data for a group of chemically related species. The thermodynamic quantities included are heat capacity, entropy, enthalpy, free energy, equilibrium constant, electrochemical potential, and relative heat content. Without further adjustment, PHAS20 will fit the model to 70 sets of data containing a total of 1200 observations on 20 species. The data may include any and all of the following types of observations:

For individual species:

1. heat capacity
2. third law entropy
3. enthalpy of formation from oxides and and elements
4. free energy of formation from oxides and elements
5. relative heat content data such as are obtained from by drop calorimetry

For reactions:

1. heat capacity change
2. entropy change
3. enthalpy change
4. enthalpy change of a transition (e.g., heat of fusion, heat of vaporization, etc.)
5. free energy change
6. equilibrium constant
7. electrochemical potential

INTRODUCTION

The ideal compilation of thermochemical data, as yet unrealized, would be both complete and accurate. The approach to completion is a function only of the assiduity of the experimentalist and is therefore beyond the reach of data compilers. Assessment of the accuracy of a thermochemical datum, however, requires knowledge of the precision of its experimental determination as well as its consistency with other equivalent measurements and with thermochemical data functionally related to it. This program automatically fits to the data a mathematical model consistent with the exact functional relations among heat capacity (Cp), entropy (S), enthalpy (H), free energy (G), equilibrium constant (K), and electrochemical potential (E) for a group of chemically related species. The program then returns a "best set" of species-related constants from which further thermodynamic calculations may be made or compilations assembled. These are accomplished by the following steps:

1. All or selected data, weighted by the reciprocal of their precision, are fitted to a mathematical model which is consistent with the thermodynamic theory for a group of chemically related species.
2. Error plots for each data set (grouped by type and reference source) are supplied.

3. The user examines the error plots and removes the discordant data sets.

4. The program is rerun and a new fit of the mathematical model to the revised data is obtained.

5. Error plots for each data set are again supplied as a check upon the decisions made in step 3.

6. Preliminary table of thermodaynamic values for each species in the chemical system is printed. As a second test, these values can be compared against existing compilation to insure all thermodynamic parameters have reasonable values.

7. At the option of the user, step-backward elimination of non-significant parameters in the mathematical model will cause repeating of steps 4, 5, and 6 for each parameter deleted. The maximum number of steps to be taken is set by the user. However, if the variance in all the parameters drops below 10 percent, elimination will also stop.

DESCRIPTION

The program PHAS20 is divided into 4 major parts; 1) data input and editing, 2) multiple regression, 3) output of error plots and associated tubular data, and 4) output of tables of preliminary thermodynamic values.

Data input and editing

The units of observations found in the literature are varied. Successful analysis requires a standard set of units. In PHAS20 the accepted units are as follows:

Parameters or Thermodynamic Property	Units
temperature	kelvin
pressure	set by user through the data selection
heat capacity	joules $mole^{-1}$ $kelvin^{-1}$
entropy	joules $mole^{-1}$ $kelvin^{-1}$
enthalpy	joules $mole^{-1}$
free energy	joules $mole^{-1}$
equilibrium constant	logarithm (base 10)
electrochemical potential	volt

Provision is made in PHAS20 to accept most data in the units given by the reference source. The temperature is edited by the following equation:

$$T\ (K) = T(\text{input}) + T(\text{factor}) \qquad (1)$$

where T(factor) is defined by the user. In most instances T(factor) will have a value 273.15 where temperatures are converted from the centigrade scale to the kelvin scale. Pressure is not an input variable. To change the units for thermodynamic properties equation 2 is used:

Y(units given in above listing) = Y(input) x Y(factor) (2)

where Y is any thermodynamic observation and Y(factor) is the conversion factor from the published units to the units used in PHAS20. This procedure simplifies input preparation because most data can be punched directly from the source and edited on input by PHAS20.

Multiple regression

Multiple regression of the mathematical model described below to the data is accomplished by the subroutines ORGLS2 and MINV20. These have been adopted from the Oak Ridge general least squares regression program by Busing and Levy (1962). The changes in the above program were those necessary to adapt it to the peculiar problem encountered here. Since all changes are superficial, the reader is referred to the report by Busing and Levy for the description of the routines.

The Mathematical Model

Thermodynamic theory provides the following exact functional relations among the heat capacity (Cp), entropy (S), enthalpy (H), free energy (G), equilibrium constant (K), and electrochemical potential (E):

$$S_i = \int \frac{Cp_i}{T} dT \tag{3}$$

$$H_i = \int Cp_i \, dT \tag{4}$$

$$G_i = H_i - T S_i \tag{5}$$

$$-R T \ln K = \sum_{i=1}^{k} s_i G_i \tag{6}$$

$$-n F E = \sum_{i=1}^{k} s_i G_i \tag{7}$$

where T is the thermodynamic temperature, R and F are the ideal gas constant and the faraday, respectively, k is the number of species in the reaction and s is the stoichiometric coefficient, positive for products and negative for reactants. From these it follows that an empirical relation which adequately defines Cp_i as a function of T will generate the mathematical description of the other thermodynamic parameters. For non-aqueous species, equation (8) has been adopted:

$$Cp_i = a_i + 2 b_i T + \frac{c_i}{T^2} + f_i T^2 + g_i / \sqrt{T} \tag{8}$$

This is an extension of the Maier-Kelley equation (Maier and Kelley, 1932), the last two terms being added to describe adequately very

accurate data.

For aqueous ions equation (9) has been adopted:

$$Cp_{i,aq} = a_i + 2b_i T + \frac{c_i}{T^2} + f_i T^2 + -g_i \frac{T}{\varepsilon} \left[\alpha^2 \exp^2 (\beta + \alpha T) + \right.$$

$$\left. \alpha^2 \exp(\beta + \alpha T) + \frac{2\alpha}{\theta} \exp(\beta + \alpha T) + \frac{1}{\theta^2} \right] \qquad (9)$$

where ε is the dielectric constant for liquid H_2O and is given by equation (10):

$$\varepsilon = \varepsilon_o \exp \left[-\exp (\beta + \alpha T) - \frac{T}{\theta}\right] \qquad (10)$$

The terms ε_o, β, α, and θ are fitted constants. Equations (9) and (10) are adopted from Helgeson (1967) but retain the original terms in the Maier-Kelley equation (the first three terms in the product of equation (9)).

Table 1 gives the mathematical model as a function of temperature describing commonly available thermodynamic observations. For further discussion the reader is referred to Fisher and Haas (1973) and subsequent reports presently in preparation.

Output of error plots and associated tabular data

After the successful multiple regression of the mathematical model to fit the data, the refined parameters are used to calculate the following statistical data for all observations in each data set:

1) difference, Y(obs)-Y(calc)
2) percent error, 100 x (Y(obs)-Y(calc))/Y(obs)
3) weighted difference, (Y(obs)-Y(calc))/standard derivation of the experimental observation
4) arithmetic mean for each of the above type of errors
5) standard error of each of 1 thru 3 about the respective means 4 for the data set.

As a guide to the quality of agreement, the weighted difference is best. The weighted difference is the number of standard errors the calculated value departs from the experimentally determined value. The weighted difference is graphed against temperature on the error plots.

The PRPLOT routine used in PHAS20 was written by Carnahan and Evans (1961).

Tables of preliminary thermodynamic values

The last portion of PHAS20 calculates and prints tables for each species in the group of the chemical system. The tables contain the following (the definition are given by the equations):

TABLE 1. THE MATHEMATICAL MODEL

A. Formulae for one nonaqueous species:

$$Cp_i = a_i + 2\,b_i T + \frac{c_i}{T^2} + f_i T^2 + \frac{g_i}{\sqrt{T}} \qquad \text{(A1)}$$

$$S_i = a_i \ln T + 2\,b_i T - \frac{c_i}{2T^2} + e_i + f_i \frac{T^2}{2} - \frac{2\,g_i}{\sqrt{T}} \qquad \text{(A2)}$$

$$H_i = a_i T + b_i T^2 - \frac{c_i}{T} + d_i + f_i \frac{T^3}{3} + 2\,g_i \sqrt{T} \qquad \text{(A3)}$$

$$G_i = a_i(T - T \ln T) - b_i T^2 - \frac{c_i}{2T} + d_i - e_i T - f_i \frac{T^3}{6} - 4\,g_i \sqrt{T} \qquad \text{(A4)}$$

B. Formulae for one aqueous species:

$$Cp_{i,aq} = a_i + 2\,b_i T + \frac{c_i}{T^2} + f_i T^2 - g_i \frac{1}{\varepsilon}\left[\alpha^2 \exp^2(\beta + \alpha T) + \alpha^2 \exp(\beta + \alpha T) + \frac{2\alpha}{\theta} \exp(\beta + \alpha T) + \frac{1}{\theta^2}\right] \qquad \text{(B1)}$$

$$S_{i,aq} = a_i \ln T + 2\,b_i T - \frac{c_i}{2T^2} + e_i + f_i \frac{T^2}{2} - g_i \frac{1}{\varepsilon}\left[\alpha \exp(\beta + \alpha T) + \frac{1}{\theta}\right] \qquad \text{(B2)}$$

$$H_{i,aq} = a_i T + b_i T^2 - \frac{c_i}{T} + d_i + \frac{f_i T^3}{3} + g_i \frac{1}{\varepsilon}\left[1 - T\,\alpha \exp(\beta + \alpha T) - \frac{T}{\theta}\right] \qquad \text{(B3)}$$

$$G_{i,aq} = a_i (T - T \ln T) - b_i T^2 - \frac{c_i}{2T} + d_i - e_i T - f_i \frac{T^3}{6} + \frac{g_i}{\varepsilon} \qquad \text{(B4)}$$

TABLE 1. Continued

$$\varepsilon = \varepsilon_o \exp[-\exp(\beta + \alpha T) \times \frac{T}{\theta}] \quad \text{(B5)}$$

($\varepsilon_o = 305.7$; $\alpha = 0.01875$; $\beta = -12.741$; $\theta = 219$)

C. Formula for relative heat content, H_R, where the ith and jth phase may be the same or different and the difference between T_2 and T_1 is the temperature interval over which the change in enthalpy is observed:

$$H_R = H_i(T_2) - H_j(T_1) \quad \text{(C1)}$$

D. Formula for a reaction involving κ species where s_i is the stoichiometric coefficient for the ith species and is positive for products and negative for reactants:

$$\Delta Cp = \sum_{i=1}^{k} s_i Cp_i \quad \text{(D1)}$$

$$\Delta S = \sum_{i=1}^{k} s_i S_i \quad \text{(D2)}$$

$$\Delta H = \sum_{i=1}^{k} s_i H_i \quad \text{(D3)}$$

$$\Delta G = \sum_{i=1}^{k} s_i G_i \quad \text{(D4)}$$

$$\log K = \frac{-1}{RT \ln(10)} \sum_{i=1}^{k} s_i G_i \quad \text{(D5)}$$

$$E = \frac{-1}{nF} \sum_{i=1}^{k} s_i G_i \quad \text{(D6)}$$

E. Constraints:

For elements in the stable structural state at 298.15 K and the pre-determined reference pressure

$$G_e \equiv 0 \equiv a_e \cdot (298.15 - 298.15 \cdot \ln 298.15) - b_e \cdot (298.15)^2 - \frac{c_e}{2 \cdot 298.15} + d_e - e_e \cdot 298.15 - \frac{f_e (298.15)^3}{6} + 4 g_e \sqrt{298.15} \quad \text{(E1)}$$

TABLE 1. Continued

For two species undergoing an isochemical phase transition at T_{tr}:

$$G_2 - G_1 \equiv (a_2-a_1)\,(T_{tr}-T_{tr}\ln T_{tr})$$
$$- (b_2-b_1)\,T_{tr}^{2}$$
$$- \frac{c_2-c_1}{2\,T_{tr}}$$
$$+ (d_2-d_1)$$
$$- (e_2-e_1)\,T_{tr}$$
$$- \frac{(f_2-f_1)\,T_{tr}^{3}}{6}$$
$$+ 4\,(g_2-g_1)\,\sqrt{T_{tr}}$$

heat capacity, $Cp(T)$

entropy, $S(T) = S_O + \int_O^T \frac{Cp}{T}\, dT$

enthalpy, $H(T) = G(T) + T\,S(T)$

free energy, $G(T) = \Delta G^\circ_{f,298} + \int_{298}^{T} Cp\, dT - T\int_{298}^{T} \frac{Cp}{T}\, dT$

equilibrium constant, $\log K = \frac{-G(T)}{2.303RT}$

electrochemical potential, $E = \frac{-G(T)}{nF}$

relative heat content, $H_R = \int_{298}^{T} Cp\, dT$

For nonaqueous species the data are calculated in the temperature range 273.15 to 2000K; for aqueous species the range is 273.15 to 523.15K. The last portion of each table contains the final constants from which the table was calculated.

Heat capacity, entropy, and relative heat content are equivalent to those given in standard compilations. The enthalpy of formation and free energy of formation of the species can be calculated provided the tables for the stable elemental species from which the species are compounded are also available;

$$\Delta G^\circ_f \text{ (species,T)} = G \text{ (species, T)} - \sum_{i=1}^{k} s_i G_i \text{ (elemental species, T)} \quad (11)$$

$$\Delta H^\circ_f \text{ (species, T)} = H \text{ (species, T)} - \sum_{i=1}^{k} s_i H_i \text{ (elemental species, T)} \quad (12)$$

where k is the number of elements in the species and s is the number of atoms of the ith element

INPUT REQUIREMENTS AND DATA DESCRIPTION

The data deck must contain the following information. Each item will be discussed in turn below.

Run data

Problem data

- Introductory data

Observations

- The Data sets
- Trial Parameters
- Plot control data

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Run Data

The introductory data in the data deck consists of two cards containing the information tabulated below. The first column gives the number of cards needed to contain the data. The second column gives the variables on the cards. The third column gives the format for each card. And the last column gives a brief description of the variables.

No. of Cards	Variable	Format	Description
1	DATE	A8	Date or other alphanumeric identification of the run.
1	NREG	I5	Number of separate problems in the data deck.

Problem Data

The data for each problem is logically broken down into four groups: 1) introductory data, 2) observations, 3) trial parameters, and 4) plot control data.

Introductory Data. The introductory data contains from 5 to 7 cards:

No. of cards	Variable	Format	Description
1	TITLE (20)	20A4	Alphanumeric description of the problem, 80 characters
1	IDO	5I5	Options: 1 for both regression and error plots, 2 for regression only, 3 for error plots only.
	NC		Maximum number of cycles or refinements permitted on trial parameters. Usually set to 2 or 3.

No. of Cards	Variable	Format	Description
	IW		Weight control options: 0 for standard errors supplied by users, 1 for uniform standard error of 1 percent to be assigned by the program (The reciprocal of the error is used as the weight on each datum).
	IL		Print control options: 0 for calculated results at plot time only, 1 for tabular data for each cycle of NC cycles.
	IFMOUT		Format control for punching of refined parameters. Options: 0 gives parameters in 6D12.5 format, 1 gives parameters in 7A8 format. Note: With IFMOUT=1, there is no round off between subsequent reruns of the same or related problems.
1	LISTP	3I5	Number of chemical species in the problem; limit is 20
	ICY		Maximum number of nonsignificant constants to be dropped by step-backward elimination.
	NHOLD		Numbers of parameters to be forced during step-backward elimination even though TEST20 may indicate they are non-significant. Limit is 40 parameters.
1-3	PNAME(LISTP)	10A8	8-character alphanumeric identification of each of the species in the chemical system.
1	ION(LISTP)	20I2	Type of species: 1 indicates a reference elemental species, 0 indicates non reference and nonaqueous species, -1 indicates aqueous species or water (H_2O liquid).

Observations. PHAS20, as described herein, will intercorrelate the type of data described by the equations in sections A, B, C, and D of Table 1. Suggestions for fitting the mathematical model to other types of data are described under Use of the Subroutine UNIQUE below.

The data may be grouped into a maximum of 70 data sets containing an aggregate of 1200 observations. These limits are set by the dimension statements and are readily changed. The grouping of data must be by identical type such as all the equilibrium constants for the same chemical reaction may be placed in one data set. But for convenience in sorting out discordant data it is recommended that such data sets be separated as to the source reference. Thus the equilibrium constants for the same reaction but from different sources should be separated into separate data sets and labeled completely on the data set identification card described below.

The Data Sets. The cards in the observation deck are as follows (Repeat beginning after the first card for each data set):

No. of Cards	Variables & Dimension Control	Format	Description
1	NSETS	I5	Number of separate data sets in the problem. Maximum set at 70.
1	REF (10, NSETS)	10A8	80-character alphanumeric description of the data in the data set.
1	NPHASE(NSETS)	6I5	Number of species described by this set. Maximum set at 6. For the heat capacity of a single phase, set to 1; for the reaction among 4 species, set to 4, etc.
	IKOUNT(NSETS)		Number of observations in the data set.
	IGO(NSETS)		Data type options (see Attachment B for examples): 1 for Cp and ΔCp, 2 for S and ΔS, 3 for H and ΔH, 4 for G and ΔG, 5 for log k, 6 for E, 7 for $H_{T_2}-H_{T_1}$, 8 thru 14 optional for situations described under Uses of the Subroutine UNIQUE.

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No. of Cards	Variable & Dimension Control	Format	Description
	ITFACT		Flag for editing of input temperatures: 0 for editing, 1 for no editing. See TFACT below.
	IPARA		Flag for editing of the dependent variable YO(I) and SIGYO(I): 0 for editing, 1 for no editing.See PARA below.
	ISIG		Flag for indicating the type of precision supplied for the observation: 0 for precision expressed as a ratio of the observed (e.g. 0.01 x YO), 1 for precision expressed as an absolute range (e.g., 0.02 J $mol^{-1}K^{-1}$).

For each of the NPHASE phases or species in the data set, prepare the following cards:

No. of Cards	Variable & Dimension Control	Format	Description
1	ANAME	(A8,2X, D10.3, 10X, 2I5)	8-character alphanumeric identifier of each species referred to in the data set. ANAME must be found in the species list PNAME, character for character and space for space
	COEF(NPHASE,NSETS)		Stoichiometric coefficient: 1) for species in reaction, positive for products, negative for reactants; or 2) number of moles upon which observation was made (generally 1 mole).
	ISTATE(NPHASE,NSETS)		Flag. If the species is a reference species with ΔG_f° at 298.15K≡0 joules per moles, set to 1. If ion or $H_2O(l)$, set to -1, otherwise set to 0.

No. of Cards	Variable & Dimension Control	Format	Description
	NINVER(NPHASE, NSETS)		Number of inversions (equals the number of lower temperature modifications being considered for the component). Maximum is 4.

If the number of inversions is zero continue with the next phase in turn or go to the next section beginning after INVPH below. If inversions are considered, insert after the phase identification card the next two cards:

No. of Cards	Variable & Dimension Control	Format	Description
1	TINV(NPHASE, NSETS, KINVER)	(4D12.5)	Inversion temperature at which ΔG(inversion) is set at 0 joules
1	INSTAT (NPHASE, NSETS)	(I5,I3, 5A8)	If a stable phase at 298.15 K is a reference species, set to 1, otherwise set to 0.
	INVSC(NPHASE NSETS)		On rare occasions there may be a stoichiometry change at a phase transformation. INVSC then contains the index of the net stoichiometry change which is found in the vector STCOEF(10) in BLOCK DATA. The reaction is: STCOEF (INVSC) PHASE1 =PHASE2.
	INVPH(NPHASE, NSETS,(KINVER + 1))		Beginning with the phase stable at 298.15K, list the succession of phases up temperature to and including the phase ANAME. (All names must be the same as found in PNAME)

After the phases and associated inversion data have been identified, give the data for the set:

No. of Cards	Variable & Dimension Control	Format	Description
IKOUNT	X(1,NO)	(6D12.5)	First independent variable, the temperature of observation.
	TFACT		Conversion factor to convert X(1,NO) (centigrade scale) to X(1,NO) (kelvin scale) by addition
	YO(NO)		Dependent variable
	PARA		Conversion factor to convert YO(NO) (any units) to YO(NO) in $J\ mol^{-1}K^{-1}$, $J\ mol^{-1}$, log K (base 10), or volts by multiplication
	SIGYO(NO)		Estimate of precision of the observation YO
	X(2,NO)		Second independent variable. For relative heat content, X(2, NO) is the reference temperature. The default is 298.15K. See Uses of the Subroutine UNIQUE for further discussion.

Repeat, beginning with REF (10,NSETS) until all data sets are entered. This then concludes the Observation portion of the input deck.

Trial Parameters. The third portions of the data deck contains the trial parameters:

No. of Cards	Variable and Dimension Control	Format	Description
1	IFMIN (LISTP)	(80I1)	Species-related flag to indicate the format used for each of LISTP species: 0 indicates (6D12 5/D12.5) 1 indicates (7A8) Because there is a format flag for each species, the format for the 7 trial parameters of one species may differ from that of the

No. of Cards	Variable and Dimension Control	Format	Description
			next. The advantage of the second format is the elimination of roundoff between runs.
1 or 2 cards per set, 1 set for each species in PNAME	P(LISTP*7)	(See IFMIN above)	Trial parameters of species sequenced as in PNAME. There are 7 parameters for each species, there must be contained on 2 cards if IFMIN=0, or 1 card if IFMIN=1. For more information on parameters, See Parameter Section below.
1 or 2	KI(LISTP*7)	(80I1)	Flag to indicate whether the parameter of the same index is to be varied during regression of kept constant: 0-to be kept constant; 1-to be varied.

If NHOLD is not zero, the next card must be included; if NHOLD is zero, the trial parameter deck is completed.

No. of Cards	Variable and Dimension Control	Format	Description
1	IHOLD(NHOLD)	(40I2)	Index of parameters in P(LISTP*7) which are to be forced to remain in regression without regard as to the statistical significance indicated by TEST20.

Plot Control Data. The plot control cards are as follows:

No. of Cards	Variable and Dimension Control	Format	Description
1	NHL	(4I5)	Number of horizontal lines in the plot less 1, generally set to 4.
	NSBH		Number of spaces between horizontal lines plus 1, generally set to 10.
	NVL		Number of vertical lines in the plot less 1. If the temperature range is 250K to 2000K, set to 7. This gives 250 degress per division.
	NSBV		Number of spaces between vertical lines plus 1. Generally set to 10.
1	XMAX	(3E10.3)	REAL*4 variable giving the upper bound on the x-coordinate.
	XMIN		REAL*4 variable giving the lower bound on the x-coordinate.
	YMAX		REAL*4 giving the upper bound on the y-coordinate. (YMIN= YMAX for a symmetrical graph). Generally set YMAX to 10.OEO. This allows weighted differences of ± 10 standard errors to be plotted, but retains enough resolution near ±1 standard error to be useful.

This concludes the deck for the plot control cards and for the problem. If more than one problem is contained in the run, the TITLE card for the next problem follows the last card above.

Choosing Trial Parameters

Equations 8 and 9 contain 5 parameters to describe the heat capacity of the ith species. In almost all situations these are more than adequate, and in most problems, using all 5 parameters will cause a singularity in the matrix inversion. For these reasons it is often best to graph the heat capacity data (or relative heat content data) to determine the parameters in the heat capacity equation (or the relative heat content equation, Section C, Table 1) which probably are adequate to describe the data. If no heat capacity or relative heat content data are available, then, at most, only "a", "d", and "e" may have

non-zero values. Some overfitting can be removed by step-backward elimination.

Because successive refinements of the parameters is a feature of ORGLS 2, order-of-magnitude estimation of trial parameters is usually sufficient. The following are acceptable first estimates for the seven parameters.

Parameter	Type of Species	
	Non-aqueous	Aqueous
a	10	10^3
b	10^{-3}	10
c	10^5	10^7
d	10^4 1/	10^5
e	10	10^4
f	10^{-7}	10^{-2}
g	10^2	10^5

Constraints

There are two preprogrammed constraints. The first deals with reference species and associated reference state, and the second with phase transformations.

Constraint derived from a reference state

The most important constraint is that the free energy of the elemental species stable at the reference temperature and reference pressure is zero. (Refer to Fisher and Haas, 1973 for a discussion of the reference state convention adopted here.) For PHAS20 TREF, the reference temperature, is set at 298.15 in BLOCK DATA. The reference pressure is never explicitly defined in PHAS20 except for aqueous species. Therefore, for non-aqueous species, the user defines the reference pressure by data selection. For aqueous species the algorithm to calculate the dielectric constant for water is applicable to vapor-saturated water only. Indirectly then, the reference pressure is a sliding reference set for ions at the coexistance curve of water.

Equation (E1) of Table 1 gives the algebraic implications of a zero free energy at a TREF of 298.15 K. Equation (13) is derived from (E1).

1/ For reference species or species related to others by phase transformation, "d" is set to zero and not varied during the regression. See Constraints below.

$$d_e = a_e(298.15 \cdot \ln(298.15) - 298.15) + b_e \cdot (298.15)^2 + \frac{c_e}{2 \cdot 298.15} + e_e \cdot 298.15 + f_e \frac{(298.15)^3}{6} - 4\, g_e (298.15)^{1/2} \quad (13)$$

In the subroutine EAFW20, for those phases specified as references (i.e. ISTATE or INSTAT = 1), d_e is calculated from TREF and the current value of the other parameters for the reference species. Therefore, in selecting trial parameters, SET D_e EQUAL TO 0.0 AND SET KI CORRESPONDING TO D_e TO 0.

Constraint derived from a phase transformation

At the temperature T_{tr} of a phase transformation the difference in the free energy between the coexiting phases is zero. This is stated algebraically by equation (E2) of Table 1. Equation (E2) can be rewritten so that d_2, the "d"-constant of the high temperature phase may be calculated from the remaining 13 constants:

$$d_2 = (a_2-a_1) \cdot (T_{tr} \cdot \ln(T_{tr}) - T_{tr}) + (b_2-b_1) \cdot T_{tr}^2 + \frac{(c_2-c_1)}{2\, T_{tr}} + d_1 + (e_2-e_1) \cdot T_{tr} + (f_2-f_1) \cdot \frac{Tr^3}{6} - 4\, (g_2-g_1) \cdot T_{tr}^{1/2} \quad (14)$$

In the subroutine EAFW20, for those phases specified as having lower temperature modifications (i.e. NINVER $\neq$ 0), d_2 is calculated from the inversion temperature T_{tr} and the current value of the other six parameters for the high temperature phase and the seven parameters for the lower temperature phase. If more than one transformation is considered, then d_1 is calculated as was d_2 using the data for successively lower temperature phases. DIMENSION statements limit the number of allowed transformations to 4.

In selecting trial parameters, SET "D" OF ALL HIGHER TEMPERATURE POLYMORPHS EQUAL TO O.O AND THE CORRESPONDING KI TO O.

Use of the Subroutine PRELIM

PRELIM is a feature retained from the program of Busing and Levy (1962). In those situations 1) where the editing feature at read-in is not sufficient to convert units or prepare the data properly for regression or 2) where a temporary adjustment in weights is desired, PRELIM can be used. PRELIM is called from the subroutine ORGLS2 just prior to the beginning of the regression procedure. Therefore PRELIM presents a last chance to make an adjustment in the data used by ORGLS2 or any subsequent routine.

As supplied, PRELIM is a dummy subroutine and returns control to ORGLS2 without any change in the data.

Use of the Subroutine UNIQUE

PHAS20 is designed to allow simultaneous regression of the mathematical model given on Table 1 to a body of experimental observations for each and all species of a chemical system. In some situations, these are observations which do not fall into any of the types given on Table 1. A regression result, to be valid, must also permit accurate calculations of the latter data. The Subroutine UNIQUE is designed to allow the user to fit the model to these data also.

By way of explanation, let us consider the following problem. In the System Sulfur at pressures less than one bar, the sum of the partial pressures of the gaseous species equals the total pressure over the condensed phase, provided the vapor obeys the ideal gas law:

$$p(\text{total}) = \sum_{j=1}^{8} p_j \qquad (15)$$

where j indicates the number of sulphur atoms in the eight polymers existing in the sulphur gas.[2/]

[2/] The species S_9, S_{10}, and S_{12} are neglected as very minor.

Equilibrium between the condensed phase and the jth gaseous species may be written

$$j\ S\ (\text{condensed}) = S_j\ (\text{ideal gas}) \qquad (16)$$

and the equilibrium constant is

$$K_j \equiv p_j \qquad (17)$$

because the activity of the condensed phase at vapor saturation is unity. Substitution of (17) into (15) gives

$$p\ (\text{total}) = \sum_{j-1}^{8} K_j \qquad (18)$$

Vapor pressure-temperature data will, therefore, provide additional constraints on the parameters a_j thru g_j which are implicit in (18).

For each datum the multiple regression routine ORGLS2 requires 1) a calculated value of the dependent variable obtained from the appropriate thermodynamic model function (i.e., the function given on Table 1), the independent variables, and the current values of the adjustable parameters a_j thru g_j and 2) the derivatives of the dependent variable with respect to each of the parameters being refined in the regression.

In cases like sulphur gas equilibria where the programmed code (given algebraically on Table 1) does not apply, the user should take the following actions:

1) Prepare the data are described under Observations above except IGO is given a value of 8 (Also 9 thru 14 are available for other constraints not included on Table 1. IGO is passed to UNIQUE in common statements and the programmer can branch in UNIQUE to the proper code to supply the requirement of 2 below).

2) The dummy routine UNIQUE is replaced by a user-coded routine UNIQUE which supplies the following:

a) YC = function (X, P) (19)

b) $DC_i = \frac{dYC}{dP_i}$ = function (X, P) (20)

where YC, X, P, and DC are, respectively, the calculated dependent variable, the independent variables, the parameters, and the derivatives of the calculated dependent variable with respect to each of the parameters. The subscript i above varies from 1 thru NP, the number of parameters in the vector P. Use of UNIQUE for vapor pressure data in the System Sulphur is given in Attachment A.

For the mathematical model given on Table 1, the data cited by 2a and 2b are already programmed in EAFW20 and the associated routines YDERIV, DDERIV, DIE, and FN.

PROGRAM RUN PREPARATION

The following deck set-up includes OS/360 control cards as well as the problem deck requirements. The program is stored on LOADLIB; the card reader/tape (SYSIN file), the line printer/tape (SYSOUT file) and the line punch (SYSOUT = B) are the required input/output devices. The OS/360 control cards are identified by //'s in columns 1-2. Each control card must be punched on an IBM 029 keypunch or equivalent card codes must be used. The symbol "␣" denotes a blank card column.

```
1  User's JOB card
2  //step␣EXEC␣PGM=G466,REGION=250K,TIME=4
3  //STEPLIB␣DD␣DSN=SYS1.LOADLIB,DISP=SHR
```

```
4  //FT06F001 DD SYSOUT=A
5  //FT07F001 DD SYSOUT=B
6  //FT05F001 DD *
7  data deck in the following order:
   run  data (2 cards)
   First Problem title (1 card)
        option codes (1 card)
        number of species, etc. (1 card)
        species names (1 to 3 cards)
        species types (1 card)
        number of data sets (1 card)
        data sets (minimum 4 cards per set; 1 reference card, 1
          option card, 1 to 6 phase cards each followed by 2
          transition data cards if applicable, and a minimum of 1
          observation card.  The maximum number of sets is 70)
        option card for trial parameter-input format (1 card)
        trial parameters (1 or 2 cards per phase depending on
          option code.)
        flags for parameters to be varied (1 or 2 cards)
        indices of parameters forced during elimination (0 or 1
          card)
        plot controls (2 cards)
   Second Problem title (1 card)
        option codes (1 card)
          .
          .
          .
          .
          plot controls (2 cards) for last problem.
8  /*
9  //
```

OUTPUT

The printed output

The printed output from PHAS20 can logically be divided into four parts, each of which will be discussed below.

1) Listing of input data sets.
2) Regression results.
) Printer plots
4) Tables of preliminary thermodynamic data and refined parameters.

For example of the printed output, refer to Attachment B.

Listing of input data sets. The first portion of the printed output contains an interpreted listing of the input data sets. The data for each set has been edited and should be in units consistent with the gas constant R and the faraday F. If this is not found to be true then the results of the regression will be of no value. The input data sets are printed by the main program PHAS20.

Regression results. The second part of the output, the results of regression begin with a listing of the regression options and the trial

parameters and ends with a listing of the correlation matrix. The regression results are printed from statements in ORGLS2 except that each reference (or data set identification) is printed from statements in EAFW20. If IL = 1, the results of all intermediate results will be printed. If IL = 0, only the references, the agreement factors, and the parameters will be printed for each refinement. The tables are self explanatory.

Printer Plots. After successful regression of the model to the data, the program forms and prints plots of the weighted difference (YO(I)-YC)/SIGYO(I) as a function of the first independent variable X(1,I). For convenience, tabular listings of the data and the difference (YO(I)-YC), the percent error (100.0 *(YO(I)-YC)/YO(I)) and the weighted difference are printed just before each error plot. The mean of the errors and the standard error about the mean are also given. The error plots plus these simple statistics are useful in sorting out discordant data sets.

The tabular data are printed from commands in the main program, PHAS20. The reference for each data set is printed by EAFW20. The printer plots are generated and printed by the entry PLOT4 of PRPLOT.

Preliminary tables of thermochemical data and the refined parameters. The last part of each problem contains tabular listings of Cp_i, S_i, H_i, G_i, log K_i, E_i and H_R as calculated from equations A1, A2, A3, A4, D5, D6, and C1 respectively. The terms log K_i, and E_i, are respectively the equilibrium constant for the formation of the ith phase at T from the elements at TREF (298.15K) and the electrochemical potential of the ith phase at T relative to the elements at TREF.

The preliminary tables are generated and printed from statements in PHAS20.

The punched output

The punched output is designed for use of the refined parameters in subsequent problems and in other programs where thermodynamic data are needed. The punched deck contains the following:

1 TITLE card for problem.
2 Number of species in problem.
3 Species name card(s). The 8-character alphanumeric name of each species in the problem.
4 The refined parameters P(LISTP*7) punched seven at a time using the format indicated by IFMOUT.
5 The complete refined parameters AA(LISTP*7) punched seven at a time using the format indicated by IFMOUT.
6 Repeat items 4 and 5 for each constant removed thru step-backward elimination.
7 Repeat items 1 thru 6 for each problem in the computer run.

In the refined parameters P(LISTP*7), the fourth parameter for each species will be zero if the species is a reference species (ISTATE = 1) or a high temperature polymorph (NINVER $\neq$ 0). To use such a set of parameters, the fourth or "d" constant must be calculated according to equations (13) and (14), respectively. This set of

parameters can be used as input into further refinements or into new regressions.

In the complete refined parameters AA(LISTP*7), the fourth parameter is zero only thru elimination. In this set, as opposed to the set above, the fourth or "d" parameter has been calculated from equations 13 and 14 where applicable. This set of parameters can be used to calculate the thermodynamic values on Table 1, sections A thru D without consideration of the reference state constraint or of the parameters of other polymorphs.

EXPLANATION OF ERROR MESSAGES

If on input, the name (8-character alphanumeric label) of a species is mispunched and cannot be found in the list of names PNAME, the computer prints "I, YOUR FRIENDLY COMPUTER, DO NOW QUIT. IN YOUR nth DATA SET YOU HAVE MISTYPED THE PHASE NAME". A comparison of the names in the nth data set with the species name cards should locate the problem. Execution of the run is terminated.

"MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PARAMETER n OF THOSE VARIED." is generated when a diagonal element of the regression matrix is zero. Find the nth element by counting the 1's in the list of KI (NP) at the beginning of the regression results until n is reached. Because the programmed derivatives in EAFW20 will not normally be zero, is wrong information stored in KI(NP)? Is a stoichiometric coefficient zero by error? Is the user-supplied UNIQUE returning a derivative DC(n) of zero? The job is terminated by this error.

"SINGULARITY RETURNED BY THE MATRIX INVERTER" indicates the matrix is singular. Most often this is caused by gross overfitting. Check whether you are likely to need all parameters. Most often, if "c_i" and "f_i" are allowed to vary simultaneously for the ith species, a singular matrix is generated. The parameter "f_i" should be used only when there is definite curvature in the heat capacity plot at the high temperature extreme. An example is found on approaching the Curie pernt or lamda pernt with rising temperature. With this error message the problem is terminated and the next problem is run.

"SUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FOR REASON 1." indicates that the change in subsequent refinements of the parameters P(I) is less than 10^{-8}. Continued refinement is generally not sound statistically. The control is returned from ORGLS2 to PHAS20 for continuation of the problem.

"***WARNING*** THE TERM SIG/(NO-NV) IS NEGATIVE. THE ABSOLUTE VALUE IS TAKEN AND THE REGRESSION CONTINUES." is self explanatory. Before you accept the results of the regression, make sure they make sense. The term SIG/(NO-NV) is used in calculating the statistics on the parameters P(NP).

"IN EAFW20 I IS GREATER THAN NO. THE NUMBER OF OBSERVATIONS. THEREFORE, I (THE COMPUTER) AM QUITTING. THE PROBLEM IS YOURS." normally cannot be generated unless NO is redefined by a user-supplied subroutine. Check common blocks in user-supplied PRELIM or UNIQUE for

NO. Make sure it was not redefined thru oversight.

"YOUR n-TH DATA SET CALLED UNIQUE FROM EAFW20, IGO(n) HAS A VALUE OF m BUT UNIQUE IS CURRENTLY UNPROGRAMMED." is most likely generated when IGO(n) has a number greater than 7 entered thru error at input. Check you data set option card. If you have programmed UNIQUE, then you may still have the dummy version in your source deck or object deck.

GLOSSARY OF MAIN FORTRAN SYMBOLS

NAME (MINIMUM DIMENSION), Definition or description

A(NPHASE, 7), In PUTOUT, local matrix containing the parameters for the data set being plotted.

A, Elsewhere, variable name assigned to the constant in the equation for the dielectric constant for water.

AA(NP), Vector containing the complete set of constants for all species in the problem.

ACOEF(NPHASE, NSETS), REAL*4 variable used for output of the coefficients of a species.

AN, The number of items in a data set.

ANAME, The name (or identification) of a species, the constants of which are constrained by the associated data set. ANAME must appear in PNAME (LISTP), character for character, blank for blank and is used to find the index of the species in PNAME. The index is then used in all subsequent calculations and is assigned to the matrix IPHASE (NPHASE, LISTP).

ASTAR, Decoration for output.

AVAL(7), REAL*4 variable used to print preliminary table of thermodynamic values.

B, Variable name assigned to the constant β in the equation for the dielectric constant for water.

BCD, LOGICAL*1 variable containing the alphanumeric character used on the printer plot.

COEF(NPHASE, NSETS), Matrix of stoichiometric coefficients for reacting species in the LISTP data sets. The coefficients are negative for reactants and positive for products by convention.

CPRIME, When the constants for the reaction are printed at plot time, the constant g is separated into g(non aqueous) and g(aqueous). CPRIME contains the g(aqueous) summation while A((NPHASE+1),7) contains the g(non aqueous) summation.

D, In PUTOUT D contains the result $d_i = a_i(T\ln T-T)+b_iT^2+C_i/2T+e_iT+f_iT^3/6-4g_iT^{1/2}$ where T=298.15, the reference temperature. The above relation is derived from the constraint (E-1) of Table 1.

DATE, 8-character alphanumeric label to identify the run. The date is suggested.

DC(NP), Vector containing the derivatives of YC with respect to the parameter P(NP).

DDDC(7), Component derivative of YC with respect to the parameters P(NP) generated by the constraints given on Table 1, section E.

DDERIV, Subroutine used to calculate DDDC.

NAME (MINIMUM DIMENSION), Definition or description

DERRP, Local variable used in TEST20.

DIE, Functions which returns the value for the dielectric constant of water at temperature T and vapor saturation.

DIEO, ε_o of the equation for the dielectric constant of water.

DYDC(7), Component of derivative of YC with respect to the parameters P(NP) at the temperature of the observation (or reference temperature for relative heat content data).

E(1), The weighted difference (YO-YC)/SIGYO passed to the printer plot routine PRPLOT.

EAFW20, Subroutine which calculates YC and DC(NP).

EBAR(3), Mean of the difference, the percent error, and the weighted difference calculated at plot time for each data set.

ERR, The difference YO-YC, REAL*4 for use in output.

ERRDP, The difference YO-YC used for calculations.

ERRP(NP), The error in P(NP) calculated in ORGLS2 and used in significance test in TEST20.

F, The faraday (96487.0 C mol^{-1}).

FN, Function returning the result FN=exp(β+αT) from the equation for the dielectric constant of water.

FNT, Result of calling FN(T).

FOUR, The value 4.0D0.

I, Local index.

ICY, Number of steps in step-backward elimination. Default = 0.

IDO, Flag to indicate operations to be executed. Options: 1 for regression and plots, 2 for regression only, 3 for plots only.

IFMIN, Flag to indicate input format for parameters P. Options: 0 for (6D12.5/D12.5), 1 for (7A8).

IFMOUT, Flag to indicate output format for parameters P. Options same as IFMIN.

IGO, Flag to indicate type of data in data set. For the types Cp, S, H, G, log K, E, and $H_{T_2}-H_{T_1}$, use 1 thru 7, respectively. For types programmed by the user in UNIQUE, use the unassigned flags 8 thru 14.

IGOES, Local variable having the value IGO+7 and used exclusively in call to YDERIV from EAFW20 or PHAS20.

IHOLD(NHOLD), Index of the parameters in P which are to remain in the regression during step-backward elimination without regard to significance.

II, Local index.

IICY, Flag to indicate the number of parameters dropped thru step-backward elimination.

IINVR, Local index.

IKOUNT(NSETS), At input, the number of observations in a data set. During run, IKOUNT contains the index of the last item in each data set.

IL, Flag to reduce print. Options: IL=0 for calculated results after cycle 3 or plot time only, IL=1 for calculated results after each refinement cycle.

NAME(MINIMUM DIMENSION), Definition or description

IMAGE(5000), LOGICAL*1 vector containing the plot image in vector form.

IN, Local index.

INDEX, Local index.

INDEX2, Local index.

INSTAT(NPHASE, NSETS), Flag to indicate whether the species stable at 298.15K is a reference species (=1) or not (=0).

INVPH(NPHASE, NSETS, NINVER), Index of the species in PNAME (LISTP) which are involved in polymorphic transitions.

INVSC (NPHASE, NSETS), If the polymorphic phase transformation at the highest temperature involves a stoichiometry change, find the appropriate reactant coefficient in the vector STCOEF and assign the index to INVSC:

Index	STCOEF
1	1.0D0
2	2.0D0
3	3.0D0
4	4.0D0
5	5.0D0
6	1/2.0D0
7	1/2.5D0
8	1/3.0D0
9	1/4.0D0
10	1/5.0D0

For example, consider the reaction: 2 $FeCl_3$(liquid) = Fe_2Cl_6 (ideal gas). Here the reactant coefficient is 2.0 and the index 2 should be assigned to INVSC.

ID, Local index.

ION (LISTP), Flag to indicate the type of species: +1 for reference species, -1 for aqueous species and H_2O(liq), 0 for all other.

IPARA, Flag to indicate whether input YO and SIGYO are to be edited IPARA=0 executes YO=YO*PARA, IPARA=1 executes no change in YO.

IPHASE(NPHASE,NSETS), Index of the names of the NPHASE species in the vector PNAME. Determined by the computer from comparison of ANAME with PNAME (LISTP).

IREDO, Index of parameter having least significance.

IREG, Local index.

ISIG, Flag to indicate whether SIGYO at input is an absolute measure (=1) or relative measure (=0) of the precision of the value of YO.

ISING, Flag to indicate singularity was found by MINV20, the matrix inverter.

ISTATE(NPHASE,NSETS), If the species is a reference species, set to 1, if the species is an ion or H_2O(liq) set to -1, otherwise set to 0.

ISTAY, Flag generated in TEST20 to indicate that at least one parameter has a percent change from the previous cycle greater than 1×10^{-6}.

ISTOP, Flag generated in TEST20 to indicate that all changes in parameters from those of the previous cycle are less than 1×10^{-6} percent. Refinement will terminate.

NAME(MINIMUM DIMENSION), Definition or description

ITFACT, Flag to indicate that the independent variables should be edited: X(J,I) = X(J,I) + TFACT.

IW, Flag: options for weighting; 0 for user supplied weights, 1 for weights uniformly set at 1 percent of observed.

IWRITE, Local flag used in EAFW20 to indicate whether a new data set is being calculated. This permits output of the data set reference.

J, Local variable.

JDFLAG, Flag to indicate whether call to UNIQUE is from ORGLS2 thru EAFW20 (JDFLAG=0) or from another routine (JDFLAG≠0). If from ORGLS2, then the derivatives DC(NP) must be supplied in addition to YC.

JN, Local index. Just before the call to ORGLS2, JN is set to zero and becomes JDFLAG in COMMON or in the arguments of the subroutines.

JO, Local index.

K, Local index.

KI(NP), Flag to indicate whether parameters are to refined (KI(I)=1), or held constant (KI(I)=0).

KINVER, Local index.

KO, Local index.

KOUNT, Local index.

L, Local index.

LABEL(NL), LOGICAL*1 Variable containing the alphanumeric legend for the ordinate of the printer plots.

LAST, Local index

LISTP, The number of species in the vector PNAME. Limit is set at 20.

LL, Local index.

LLL, Local index.

LST, Local index.

LSTINV, Local index.

LSTPHA, Local index.

M, Local index.

NC, The number of refinement cycles to be taken by ORGLS2. Generally set to 2 or 3.

NDATA, The number of items in a data set.

NHL, The number of horizontal lines on the printer plot less 1.

NHOLD, The number of parameters to be forced to remain in the regression without regard to the results of TEST20.

NINVER(NPHASE,NSETS), The number of phase transitions which occur in the chemical component between the temperature of the observation X(1,I) and the reference temperature for the elements at 298.15K.

NL, The number of characters in the legend LABEL.

NO, The total number of observations in the problem. Limit is 1200 observations total.

NOYES, Local index.

NP, The numbers of parameters. The limit is set at 140.

NPHAS, Local index.

NPHASE(NSETS), The number of species in the jth set of data.

NREG, The number of problems in the computer run. No limit.

NAME(MINIMUM DIMENSION), Definition or description

NSBH, The number of spaces between the horizontal lines plus 1 on the printer plot.

NSBV, The number of spaces between vertical lines plus 1 on the printer plot.

NSCALE(5), Arguments used to set up the image by the routine PRPLOT. Here all values are set to zero.

NSETS, The numbers of data sets in a problem. Limit is 70 data sets in a problem.

NP, The number of parameters being varied (i.e., KI(I)=1).

NX, The number of independent variables. Limit set at 2.

ONE, The constant 1.0D0.

ORGLS2, Revision of the program OR GLS by Busing and Levy (1962) designed for the peculiar needs of PHAS20.

P(LISTP*7), Parameters for the species.

PARA, Input variable used in editing the dependent variable YO.

PD(NV), Calculated parameter changes for those parameters which are changed.

PHINV(NINVER+1), 8-character alphanumeric labels for each phase in inversion sequence. Begin with the phase stable at 298.15K and progress to include the phase stable at the temperature of observation.

PLOT1, ENTRY points into the routine PRPLOT.
$PLOT_2$
$PLOT_3$
$PLOT_4$

PNAME(LISTP), 8-character alphanumeric labels for each species in the problem.

PUTOUT, Routine called at plot time to calculate the complete set of constants, including "d_i" if constraints are applicable.

R, The gas constant (8.3142 J $mol^{-1}K^{-1}$) times ln(10) = 19.144379D0.

REF(10,NSETS), 80 character alphanumeric label for each data set.

RELERR, Local variable giving the percent error of each calculated value relative to the observed data.

SC, Local variable containing the stoichiometric variable.

SCINV(2), Constants: -1.0D0, +1.0D0.

SERR(3), The 3 sums-of-errors for a data set.

SERRSQ(3), The 3 sums-of-errors-squared for a data set.

SGN(2), Local variable used during the calculation of "d_i" which is derived from the other parameters because of constraints.

SIGYO(NO), The standard error of an observation YO(I). The reciprocal is used as the weight.

SIX, The constant 6.0D0.

STCOEF(10), Vector of possible stoichiometric coefficients for a change in stoichiometry at a phase transformation. Refer to INVSC above.

STDEV(3), The standard error of the data about the mean error EBAR for a data set.

T, Local variable.

NAME(MINIMUM DIMENSION), Definition or description

TEST20, Routine which does the following: 1) Signals the end of refinement cycling if the percent change in a parameter is less than 10^{-6}, 2) Locates the least significant parameter being refined but not constrained by IHOLD to stay in step-backward elimination, 3) Signals the end of step-backward elimination if the error on all parameters is less than 10 percent.

TFACT, Local input variable used in editing X(J,I) by addition.

THETA, The constant θ of the equation for the dielectric constant of water.

THREE, The constant 3.0D0.

TINV(NPHASE,NSETS,NINVER), The inversion temperatures beginning with the closest temperature to 298.15K.

TITLE(20), 80 character alphanumeric label for the problem.

TK(19,2), Array of temperatures used to calculate the preliminary tables of thermodynamic constants for a species.

TO, Local variable.

TREF, The constant 298.15 which is the reference temperature from the reference state convention.

TWO, The constant 2.0D0.

TYPE, Legends for output of data type.

UNIQUE, Subroutine to be programmed by user if data not considered on Table 1 are available and used in refinement. Refer to Use of the Subroutine UNIQUE.

UNITS, 8 character alphanumeric label for the type of energy data consistent with R and F. As supplied, UNITS has the label 'JOULES'.

VAL(7), Local variables.

X(2,NO), The independent variable. X(1,NO) is the absolute temperature. X(2,NO) is an optional second independent variable used in the current code for the reference temperature of relative heat content data.

XI(1), REAL*4 variable containing the x-coordinate of the datum being passed to the routine PRPLOT.

XMIN, The lowest temperature for the error plot.

XMAX, The highest temperature for the error plot

YC, The value of the dependent variable calculated from the current set of parameters.

YDERIV, Routine which calculates the temperature-dependent part of the derivative $d\,YC/d\,P_i$

YESNO(2), The labels 'YES' and 'NO' used in printing input data.

YMAX, The upper bound of the y-axis on the error plot. YMAX= -YMIN.

YMIN, The lower bound of the y-axis on the error plot. YMIN= -YMAX.

YO(NO), The dependent variable.

ZERO, The constant 0.0D0.

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ATTACHMENT A

Example of the Use of the Subroutine UNIQUE

In the text, there is a discussion of the use of the Subroutine UNIQUE with the System Sulfur given as an example. The attached routines UNIQUE, VPRESS, and KJCALC will provide values for YC and DC(NP) for an IGO of 8.

The subroutine UNIQUE calls the appropriate subroutine VPRESS when IGO for the data set is 8. If IGO of the data set is 9, 10, 11 or 12, subroutines SNCOEF, ACTSUL, INFLO, and ININT are called. These are not given, but would contain other constraints on the parameters for the gaseous species in the System Sulfur.

The subroutine KJCALC is a modified version of EAFW20 and returns the eight constants KJ for reaction 16 of the text. KJCALC also generates the data for the matrix TDC(8,NP), the derivatives of each equilibrium constant with respect to the NP parameters of the vector P.

The subroutine VPRESS calculates YC and DN(NP) by summing KJ(8) and TDC(8,NP) for the eight reactions.

```
      SUBROUTINE UNIQUE (YC,N,JO,JDFLAG)                                UNI  10
      IMPLICIT REAL*8(A-H,C-Z)                                          UNI  20
      DIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),         UNI  30
     I  NPHASE(70),IKOUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),        UNI  40
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                         UNI  50
      COMMON /EARTHA COEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGC,NSETS,    UNI  60
     1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                         UNI  70
      M=IGC(JO)-7                                                       UNI  80
      GO TO (100,200,300,400,500), M                                    UNI  90
  100 CONTINUE                                                          UNI 100
      CALL VPRESS (YC,N,JO,JDFLAG)                                      UNI 110
      RETURN                                                            UNI 120
  200 CONTINUE                                                          UNI 130
      CALL SNCOEF (YC,N,JO,JDFLAG)                                      UNI 140
      RETURN                                                            UNI 150
  300 CONTINUE                                                          UNI 160
      CALL ACTSLL (YC,N,JO,JDFLAG)                                      UNI 170
      RETURN                                                            UNI 180
  400 CONTINUE                                                          UNI 190
      CALL INFLC (YC,N,JO,JDFLAG)                                       UNI 200
      RETURN                                                            UNI 210
  500 CONTINUE                                                          UNI 220
      CALL ININT (YC,N,JO,JDFLAG)                                       UNI 230
      RETURN                                                            UNI 240
      END                                                               UNI 250-
```

```
      SUBROUTINE VPRESS (YC,I,JO,JCFLAG)                                VPR  10
      IMPLICIT REAL*8(A-H,O-Z)                                          VPR  20
      REAL*4 TITLE(20)                                                  VPR  30
      REAL*8 LOCK(8),KJ(8)                                              VPR  40
      DIMENSION TDC(8,140)                                              VPR  50
      DIMENSION X(2,1200),YC(1200),SIGYC(1200),P(140),KI(140),          VPR  60
     1  DC(140),PC(140)                                                 VPR  70
      COMMON /AIR/ X, P, DC, TITLE, YG, SIGYC, PC, KI, NC, NV, NX, IW,  VPR  80
     I  NP, NO, ISING, ISTOP, IL                                        VPR  90
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F              VPR 100
      COMMON /BPIM/LOCK,KJ,TDC                                          VPR 110
      YC=ZERO                                                           VPR 120
      T=X(I,1)                                                          VPR 130
      CALL KJCALC (T,JO)                                                VPR 140
      DO 100 J=2,8                                                      VPR 150
      YC=YC+KJ(J)                                                       VPR 160
  100 CONTINUE                                                          VPR 170
      IF (JCFLAG.NE.0) RETURN                                           VPR 180
      DO 200 K=I,NP                                                     VPR 190
      DO 200 J=2,8                                                      VPR 200
      DC(K)=DC(K)+TDC(J,K)                                              VPR 210
  200 CONTINUE                                                          VPR 220
      RETURN                                                            VPR 230
      END                                                               VPR 240
```

```
      SUBROUTINE KJCALC (T,J)                                          KJC  10
      IMPLICIT REAL*8(A-H,O-Z)                                         KJC  20
      DIMENSION SGN(2),CC(140)                                         KJC  30
      DIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),        KJC  40
     1  NPHASE(70),IKCUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),       KJC  50
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                         KJC  60
      REAL*4 TITLE(20)                                                 KJC  70
      DIMENSION X(2,1200),YC(1200),SIGYO((200),F(140),KI(140),         KJC  80
     1  ZZ(140),PO(140)                                                KJC  90
      DIMENSION REF(10,70),ERRP(140)                                   KJC 100
      DIMENSION DCOC(7),OYCC(7)                                        KJC 110
      DIMENSION SCINV(2),STCOEF(10)                                    KJC 120
      REAL*8 LOGK(8),KJ(8)                                             KJC 130
      DIMENSION TDC(8,140)                                             KJC 140
      COMMON /EARTH/ COEF,PNAME,TINV,IPHASE,NPHASE,IKCUNT,IGO,NSETS,   KJC 150
     1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                         KJC 160
      COMMON /AIR/ X, P, ZZ, TITLE, YC, SIGYO, PO, KI, NO, NV, NX, IW, KJC 170
     1  NP, ND, ISING, ISTOP, IL, JOBFLAG                              KJC 180
      COMMON /FIRE/ REF, ERRP, IMPRIN, ICY, IICY, IPOOC                KJC 190
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,            KJC 200
     1  SCINV, TREF, STCOEF                                            KJC 210
      COMMON /SPACE/ DCOC, OYOC, SC, TC                                KJC 220
      COMMON /BRIM/LOGK,KJ,TDC                                         KJC 230
      COMMON /WOMAN/LNIC,LOGE                                          KJC 240
      CALL YDERIV (T,5)                                                KJC 250
      IF ((GO(J).NE.12) GO TO 100                                      KJC 260
      M1=IPHASE(3,J)                                                   KJC 270
      M2=IPHASE(3,J)                                                   KJC 280
      GO TO 200                                                        KJC 290
  100 CONTINUE                                                         KJC 300
      M1=2                                                             KJC 310
      M2=8                                                             KJC 320
  200 CONTINUE                                                         KJC 330
      DO 1800 M=M1,M2                                                  KJC 340
      DO 300 K=1,NP                                                    KJC 350
      DC(K)=ZERO                                                       KJC 360
      TDC(M,K)=ZERO                                                    KJC 370
  300 CONTINUE                                                         KJC 380
      LOGK(M)=ZERO                                                     KJC 390
      NTEMP=NPHASE(J)                                                  KJC 400
      NPHASE(J)=2                                                      KJC 410
      IPHASE(2,J)=M                                                    KJC 420
      COEF(1,J)=-M                                                     KJC 430
      COEF(2,J)=1                                                      KJC 440
      ISTATE(2,J)=0                                                    KJC 450
      NINVER(2,J)=0                                                    KJC 460
      LAST=NPHASE(J)                                                   KJC 470
      DO 150 L=1,LAST                                                  KJC 480
      INDEX=1+7*(IPHASE(L,J)-1)                                        KJC 490
      SC=COEF(L,J)                                                     KJC 500
      IF (ISTATE(L,J).NE.1) GO TO 500                                  KJC 510
      CALL ODERIV (TREF)                                               KJC 520
      DO 400 K=1,7                                                     KJC 530
      CC(K+INDEX-1)=CC(K+INDEX-1)+SC*DCOC(K)*OYCC(4)                   KJC 540
  400 CONTINUE                                                         KJC 550
      GO TO 1300                                                       KJC 560
  500 CONTINUE                                                         KJC 570
      IF (NINVER(L,J).LE.0) GO TO 1300                                 KJC 580
      DO 600 LLL=1,2                                                   KJC 590
      SGN(LLL)=SCINV(LLL)                                              KJC 600
```

```
  600 CONTINUE                                                          KJC 610
      IF (INVSC(L,J).EQ.0) GO TO 700                                    KJC 620
      SGN(1)=SGN(1)*STCOEF(INVSC(L,J))                                  KJC 630
      SGN(2)=SGN(2)*STCOEF(INVSC(L,J))                                  KJC 640
  700 CONTINUE                                                          KJC 650
      IF (INSTAT(L,J).EQ.0) GO TO 900                                   KJC 660
      IINVR=1+7*(INVPH(L,J,1)-1)                                        KJC 670
      CALL DDERIV (TREF)                                                KJC 680
      DO 800 K=1,7                                                      KJC 690
      DC(K+IINVR-1)=DC(K+IINVR-1)+DDOC(K)*SGN(2)*SC*DYDC(4)             KJC 700
  800 CONTINUE                                                          KJC 710
  900 CONTINUE                                                          KJC 720
      LSTINV=NINVER(L,J)                                                KJC 730
      DO 1200 LL=1,LSTINV                                               KJC 740
      CALL DDERIV (TINV(L,J,LL))                                        KJC 750
      IF (INVSC(L,J).EQ.0) GO TO 1000                                   KJC 760
      IF (LL.NE.LSTINV) GO TO 1000                                      KJC 770
      SGN(2)=SGN(2)/STCOEF(INVSC(L,J))                                  KJC 780
 1000 CONTINUE                                                          KJC 790
      DO 1100 LLL=1,2                                                   KJC 800
      IINVR=1+7*(INVPH(L,J,(LL+LLL-1))-1)                               KJC 810
      DO 1100 K=1,7                                                     KJC 820
      DC(K+IINVR-1)=DC(K+IINVR-1)+DDOC(K)*SGN(LLL)*SC*DYDC(4)           KJC 830
 1100 CONTINUE                                                          KJC 840
 1200 CONTINUE                                                          KJC 850
 1300 CONTINUE                                                          KJC 860
      DO 1400 K=1,7                                                     KJC 870
      DC(K+INDEX-1)=DC(K+INDEX-1)+SC*DYDC(K)                            KJC 880
 1400 CONTINUE                                                          KJC 890
 1500 CONTINUE                                                          KJC 900
      DO 1600 K=1,NP                                                    KJC 910
      LOGK(M)=LOGK(M)+P(K)*DC(K)                                        KJC 920
 1600 CONTINUE                                                          KJC 930
      IF (LOGK(M).GT.7.585901) GO TO 1900                               KJC 940
      KJ(M)=1.0D1**LOGK(M)                                              KJC 950
      DO 1700 K=1,NP                                                    KJC 960
      TDC(M,K)=TDC(M,K)+KJ(M)*LN10*DC(K)                                KJC 970
 1700 CONTINUE                                                          KJC 980
 1800 CONTINUE                                                          KJC 990
      NPHASE(J)=NTEMP                                                   KJC1000
      COEF(1,J)=ONE                                                     KJC1010
      RETURN                                                            KJC1020
 1900 CONTINUE                                                          KJC1030
      WRITE (6,2000) M,LOGK(M)                                          KJC1040
      STOP                                                              KJC1050
 2000 FORMAT ('0FOR YOUR',I2,'-TH SPECIES, YOU HAVE TRIED TO CALCULATE 1KJC1060
     10.0**',D12.5,'.'/' I JUST CANNOT HACK SUCH LARGE NUMBERS.  IT IS TKJC1070
     2IRING ON THE BRAIN.')                                             KJC1080
      END                                                               KJC1090-
```

ATTACHMENT B

EXAMPLES OF AN EXECUTION OF PHAS20

Problem 1. The System H_2O and the self-ionization of water

Consider the System H_2O including the self-ionization of liquid H_2O(water). There are four species:

H_2O(ideal gas)
H_2O(liquid, i.e. water)
H^+(aqueous hydrated ion)
OH^-(aqueous hydrated ion)

In considering this chemical system, the constants for H_2O(ideal gas) are based upon an earlier run and are not further refined here; the constants for H_2O(liquid), H^+(aq), and OH^-(aq) are sought. Only the following portion of the data available are used in the refinement to keep the problem in manageable bounds for publication:

1. The equilibrium constant reaction H_2O(liquid) = H_2O(ideal gas).
2. The relative heat content data for liquid H_2O.
3. ΔCp for the self-ionization of liquid H_2O.
4. ΔH for the self-ionization of liquid H_2O.
5. Selected equilibrium constants for the self-ionization of liquid H_2O.

The following pages give the listing of the input and output for the regression of the model to these data.

Listing of input deck. The next four pages contain a listing of the input deck. Deleted from the input are the constants for H_2O(G) which were in the format (7A8).

```
10/31/73
    1
PROBLEM 1,  THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.
    1    3    0    1    1
    4    0    0
H2O  (G)H2O  (L)H+      OH-
 0-1-1-1
    6
H2O(L)  =  H2O(G),LOG K.                    HAAS, 1970
    2   36    5    0    1    1
H2O  (G)   1.0000 00                  0     0
H2O  (L)  -1.0000 00                 -1     0
   0.010D 00 273.150D 00-2.21970D 00                0.008000D 00
  10.000D 00 273.150D 00-1.91720D 00                0.004000D 00
  20.000D 00 273.150D 00-1.63760D 00                0.004000D 00
  30.000D 00 273.150D 00-1.37880D 00                0.004000D 00
  40.000D 00 273.150D 00-1.13900D 00                0.004000D 00
  50.000D 00 273.150D 00-0.91610D 00                0.004000D 00
  60.000D 00 273.150D 00-0.70850D 00                0.004000D 00
  70.000D 00 273.150D 00-0.51500D 00                0.004000D 00
  80.000D 00 273.150D 00-0.33410D 00                0.004000D 00
  90.000D 00 273.150D 00-0.16490D 00                0.004000D 00
 100.000D 00 273.150D 00-0.00630D 00                0.004000D 00
 110.000D 00 273.150D 00 0.14240D 00                0.005000D 00
 120.000D 00 273.150D 00 0.28220D 00                0.006000D 00
 130.000D 00 273.150D 00 0.41380D 00                0.007000D 00
 140.000D 00 273.150D 00 0.53760D 00                0.008000D 00
 150.000D 00 273.150D 00 0.65440D 00                0.009000D 00
 160.000D 00 273.150D 00 0.76470D 00                0.010000D 00
 170.000D 00 273.150D 00 0.86890D 00                0.011000D 00
 180.000D 00 273.150D 00 0.96740D 00                0.012000D 00
 190.000D 00 273.150D 00 1.06060D 00                0.012000D 00
 200.000D 00 273.150D 00 1.14890D 00                0.013000D 00
 210.000D 00 273.150D 00 1.23270D 00                0.014000D 00
 220.000D 00 273.150D 00 1.31220D 00                0.015000D 00
 230.000D 00 273.150D 00 1.38860D 00                0.015000D 00
 240.000D 00 273.150D 00 1.45940D 00                0.016000D 00
 250.000D 00 273.150D 00 1.52760D 00                0.016000D 00
 260.000D 00 273.150D 00 1.58600D 00                0.017000D 00
 270.000D 00 273.150D 00 1.65420D 00                0.017000D 00
 280.000D 00 273.150D 00 1.71310D 00                0.018000D 00
 290.000D 00 273.150D 00 1.76820D 00                0.018000D 00
 300.000D 00 273.150D 00 1.82270D 00                0.019000D 00
 310.000D 00 273.150D 00 1.87380D 00                0.019000D 00
 320.000D 00 273.150D 00 1.92270D 00                0.019000D 00
 330.000D 00 273.150D 00 1.96940D 00                0.020000D 00
 340.000D 00 273.150D 00 2.01490D 00                0.020000D 00
 350.000D 00 273.150D 00 2.05700D 00                0.020000D 00
H2O  (L), H(T)-H(273.16)                    OSBORNE, STIMSON, AND GINNINGS, 1939
    2   73    7    0    0    0
H2O  (L)   1.000D 00                 -1     0
H2O  (L)  -1.000D 00                 -1     0
   5.000D 00 273.150D 00   5.028D 00 1.800660D 01 0.000500D 00 0.010000D 00
  10.000D 00 273.150D 00  10.040D 00 1.800660D 01 0.000500D 00 0.010000D 00
  15.000D 00 273.150D 00  15.043D 00 1.800660D 01 0.000500D 00 0.010000D 00
  20.000D 00 273.150D 00  20.040D 00 1.800660D 01 0.000500D 00 0.010000D 00
  25.000D 00 273.150D 00  25.033D 00 1.800660D 01 0.000500D 00 0.010000D 00
  30.000D 00 273.150D 00  30.024D 00 1.800660D 01 0.000500D 00 0.010000D 00
  35.000D 00 273.150D 00  35.015D 00 1.800660D 01 0.000500D 00 0.010000D 00
  40.000D 00 273.150D 00  40.006D 00 1.800660D 01 0.000500D 00 0.010000D 00
```

```
 45.0000 00 273.1500 00   44.9970 00 1.8000660 01 0.0000500 00 0.0100000 00
 50.0000 00 273.1500 00   49.9900 00 1.8000660 01 0.0000500 00 0.0100000 00
 55.0000 00 273.1500 00   54.9840 00 1.8000660 01 0.0000500 00 0.0100000 00
 60.0000 00 273.1500 00   59.9810 00 1.8000660 01 0.0000500 00 0.0100000 00
 65.0000 00 273.1500 00   64.9810 00 1.8000660 01 0.0000500 00 0.0100000 00
 70.0000 00 273.1500 00   69.9840 00 1.8000660 01 0.0000500 00 0.0100000 00
 75.0000 00 273.1500 00   74.9910 00 1.8000660 01 0.0000500 00 0.0100000 00
 80.0000 00 273.1500 00   80.0020 00 1.8000660 01 0.0000500 00 0.0100000 00
 85.0000 00 273.1500 00   85.0180 00 1.8000660 01 0.0000500 00 0.0100000 00
 90.0000 00 273.1500 00   90.0390 00 1.8000660 01 0.0000500 00 0.0100000 00
 95.0000 00 273.1500 00   95.0670 00 1.8000660 01 0.0000500 00 0.0100000 00
100.0000 00 273.1500 00  100.1020 00 1.8000660 01 0.0000500 00 0.0100000 00
105.0000 00 273.1500 00  105.1430 00 1.8000660 01 0.0000500 00 0.0100000 00
110.0000 00 273.1500 00  110.1930 00 1.8000660 01 0.0000500 00 0.0100000 00
115.0000 00 273.1500 00  115.2500 00 1.8000660 01 0.0000500 00 0.0100000 00
120.0000 00 273.1500 00  120.3200 00 1.8000660 01 0.0000500 00 0.0100000 00
125.0000 00 273.1500 00  125.4000 00 1.8000660 01 0.0000500 00 0.0100000 00
130.0000 00 273.1500 00  130.4900 00 1.8000660 01 0.0000500 00 0.0100000 00
135.0000 00 273.1500 00  135.6000 00 1.8000660 01 0.0000500 00 0.0100000 00
140.0000 00 273.1500 00  140.7200 00 1.8000660 01 0.0000500 00 0.0100000 00
145.0000 00 273.1500 00  145.8500 00 1.8000660 01 0.0000500 00 0.0100000 00
150.0000 00 273.1500 00  151.0000 00 1.8000660 01 0.0000500 00 0.0100000 00
155.0000 00 273.1500 00  156.1600 00 1.8000660 01 0.0000500 00 0.0100000 00
160.0000 00 273.1500 00  161.3400 00 1.8000660 01 0.0000500 00 0.0100000 00
165.0000 00 273.1500 00  166.5500 00 1.8000660 01 0.0000500 00 0.0100000 00
170.0000 00 273.1500 00  171.7700 00 1.8000660 01 0.0000500 00 0.0100000 00
175.0000 00 273.1500 00  177.0100 00 1.8000660 01 0.0000500 00 0.0100000 00
180.0000 00 273.1500 00  182.2800 00 1.8000660 01 0.0000500 00 0.0100000 00
185.0000 00 273.1500 00  187.5700 00 1.8000660 01 0.0000500 00 0.0100000 00
190.0000 00 273.1500 00  192.8800 00 1.8000660 01 0.0000500 00 0.0100000 00
195.0000 00 273.1500 00  198.2300 00 1.8000660 01 0.0000500 00 0.0100000 00
200.0000 00 273.1500 00  203.5900 00 1.8000660 01 0.0000500 00 0.0100000 00
205.0000 00 273.1500 00  209.0300 00 1.8000660 01 0.0000500 00 0.0100000 00
210.0000 00 273.1500 00  214.4300 00 1.8000660 01 0.0000500 00 0.0100000 00
215.0000 00 273.1500 00  219.9300 00 1.8000660 01 0.0000500 00 0.0100000 00
220.0000 00 273.1500 00  225.4000 00 1.8000660 01 0.0000500 00 0.0100000 00
225.0000 00 273.1500 00  230.9500 00 1.8000660 01 0.0000500 00 0.0100000 00
230.0000 00 273.1500 00  236.5300 00 1.8000660 01 0.0000500 00 0.0100000 00
235.0000 00 273.1500 00  242.1600 00 1.8000660 01 0.0000500 00 0.0100000 00
240.0000 00 273.1500 00  247.8400 00 1.8000660 01 0.0000500 00 0.0100000 00
245.0000 00 273.1500 00  253.5700 00 1.8000660 01 0.0000500 00 0.0100000 00
250.0000 00 273.1500 00  259.3500 00 1.8000660 01 0.0000500 00 0.0100000 00
255.0000 00 273.1500 00  265.1900 00 1.8000660 01 0.0000500 00 0.0100000 00
260.0000 00 273.1500 00  271.0900 00 1.8000660 01 0.0000500 00 0.0100000 00
265.0000 00 273.1500 00  277.0600 00 1.8000660 01 0.0000500 00 0.0100000 00
270.0000 00 273.1500 00  283.0900 00 1.8000660 01 0.0000500 00 0.0100000 00
275.0000 00 273.1500 00  289.2100 00 1.8000660 01 0.0000500 00 0.0100000 00
280.0000 00 273.1500 00  295.4100 00 1.8000660 01 0.0000500 00 0.0100000 00
285.0000 00 273.1500 00  301.7000 00 1.8000660 01 0.0000500 00 0.0100000 00
290.0000 00 273.1500 00  308.1000 00 1.8000660 01 0.0000500 00 0.0100000 00
295.0000 00 273.1500 00  314.6000 00 1.8000660 01 0.0000500 00 0.0100000 00
300.0000 00 273.1500 00  321.2200 00 1.8000660 01 0.0000500 00 0.0100000 00
305.0000 00 273.1500 00  327.9800 00 1.8000660 01 0.0000500 00 0.0100000 00
310.0000 00 273.1500 00  334.8900 00 1.8000660 01 0.0000500 00 0.0100000 00
315.0000 00 273.1500 00  341.9700 00 1.8000660 01 0.0000500 00 0.0100000 00
320.0000 00 273.1500 00  349.2400 00 1.8000660 01 0.0000500 00 0.0100000 00
325.0000 00 273.1500 00  356.7300 00 1.8000660 01 0.0000500 00 0.0100000 00
330.0000 00 273.1500 00  364.4800 00 1.8000660 01 0.0000500 00 0.0100000 00
335.0000 00 273.1500 00  372.5400 00 1.8000660 01 0.0000500 00 0.0100000 00
340.0000 00 273.1500 00  380.9300 00 1.8000660 01 0.0000500 00 0.0100000 00
345.0000 00 273.1500 00  389.7600 00 1.8000660 01 0.0000500 00 0.0100000 00
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 350.0000 00 273.1500 00 399.1730 00 1.800660 01 0.000500 00 0.010000 00
 355.0000 00 273.1500 00 409.3630 00 1.800660 01 0.000500 00 0.010000 00
 360.0000 00 273.1500 00 420.7400 00 1.800660 01 0.000500 00 0.010000 00
 365.0000 00 273.1500 00 434.1200 00 1.800660 01 0.000500 00 0.010000 00
H+ + OH- = H2O(L), DELTA CP, REACTION.  ACKERMANN, 1958.
    3    4    1    0    1    1
H2O  (L)   1.0000 00              -1    0
H+        -1.0000 00              -1    0
OH-       -1.0000 00              -1    0
  10.0000 00 273.1500 00 69.20000 00                3.000000 00
  30.0000 00 273.1500 00 50.10000 00                3.000000 00
  50.0000 00 273.1500 00 41.80000 00                3.000000 00
  70.0000 00 273.1500 00 42.30000 00                3.000000 00
H2O = OH- + H+, HEAT OF IONIZATION      OLOFSSON AND OLOFSSON, 1973.
    3    6    3    1    0    1
H2O  (L)  -1.0000 00              -1    0
H+         1.0000 00              -1    0
OH-        1.0000 00              -1    0
 298.1500 00              55.92000 032.3900570-01 0.020000 03
 323.1500 00              50.92000 032.3900570-01 0.020000 03
 347.5500 00              46.67000 032.3900570-01 0.020000 03
 373.5500 00              42.67000 032.3900570-01 0.020000 03
 398.4500 00              37.35000 032.3900570-01 0.020000 03
 417.7500 00              33.45000 032.3900570-01 0.020000 03
 LOG KW                                BIGNOLD, BREWER, AND HEARN, 1971.
    3   24    5    0    1    1
H2O  (L)  -1.0000 00              -1    0
H+         1.0000 00              -1    0
OH-        1.0000 00              -1    0
  51.0000 00 273.1500 00-13.24100 00                0.021000 00
  60.9000 00 273.1500 00-12.99190 00                0.021000 00
  70.5000 00 273.1500 00-12.80160 00                0.013000 00
  80.2000 00 273.1500 00-12.64170 00                0.010000 00
  89.9000 00 273.1500 00-12.49000 00                0.028000 00
  99.3000 00 273.1500 00-12.23430 00                0.039000 00
 108.6000 00 273.1500 00-12.07450 00                0.025000 00
 118.0000 00 273.1500 00-11.96640 00                0.014000 00
 127.3000 00 273.1500 00-11.86990 00                0.014000 00
 136.7000 00 273.1500 00-11.76720 00                0.020000 00
 146.0000 00 273.1500 00-11.72080 00                0.024000 00
 155.4000 00 273.1500 00-11.60760 00                0.017000 00
 164.7000 00 273.1500 00-11.54770 00                0.015000 00
 174.2000 00 273.1500 00-11.47280 00                0.008000 00
 183.6000 00 273.1500 00-11.39290 00                0.008000 00
 193.0000 00 273.1500 00-11.33260 00                0.014000 00
 202.5000 00 273.1500 00-11.27900 00                0.008000 00
 212.1000 00 273.1500 00-11.25860 00                0.008000 00
 221.7000 00 273.1500 00-11.22830 00                0.008000 00
 231.4000 00 273.1500 00-11.21550 00                0.008000 00
 241.2000 00 273.1500 00-11.20210 00                0.008000 00
 251.0000 00 273.1500 00-11.19560 00                0.009000 00
 261.0000 00 273.1500 00-11.20390 00                0.009000 00
 271.0000 00 273.1500 00-11.21970 00                0.017000 00
H2O = OH- + H+, LOG KW.                 SWEETON, MESMER & BAES, PERS COMM, 1973.
    3    7    5    0    1    1
H2O  (L)  -1.0000 00              -1    0
H+         1.0000 00              -1    0
OH-        1.0000 00              -1    0
    0.000 00 273.1500 00-14.94100 00                0.009000 00
   50.000 00 273.1500 00-13.27200 00                0.006000 00
  100.000 00 273.1500 00-12.26400 00                0.009000 00
```

```
  150.000 00 273.1500 00-11.64200 00                0.012000 00
  200.000 00 273.1500 00-11.30200 00                0.012000 00
  250.000 00 273.1500 00-11.19600 00                0.015000 00
  300.000 00 273.1500 00-11.30100 00                0.045000 00
(A-FORMATED CONSTANTS FROM RUN ON 10/13/73.  NOT LISTED)        10/13/73H2O   (G)
 2.356790 01-1.728260-02 0.0        -5.76916D 04-1.097180 02 5.242220-05H2O   (L)
-1.069550 03                                                          H2O   (L)
 0.0          0.0          0.0          0.0          0.0          0.0         H+
 0.0                                                                         H+
 3.080590 02-3.058170-01-1.398640 07-1.498200 05-1.65259D 03 0.0          OH-
 0.0                                                                         OH-
0000000110111100000001111100
    4   10    8   10
673.15D 00273.150 00 1.0000 01
```

Printed output. The following pages contain a complete printed output from the execution of PHAS20 using the preceding data deck.

U. S. GOVERNMENT PRINTING OFFICE : 1972 O - 481 084

THESE RESULTS WERe OBTAINED IN A RUN ON 10/31/73

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

PHASES CONSIDERED IN THIS REGRESSION ARE AS FOLLOWS---

H2O (G) H2O (L) H+ OH-

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

10/31/73

THE FOLLOWING DATA SETS HAVE BEEN READ IN TO STORAGE:

SET NUMBER REFERENCE

****

1 H2O(L) = H2O(G),LOG K. HAAS, 1970

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 36
THE TYPE OF DATA IS: LOG K

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
H2O (G)	1.000	NO	0
H2O (L)	-1.000	NO	0

INDEX	TEMPERATURE T2	T1	LOG K	ERROR
1	273.160	-	-2.219700 00	8.000000-03
2	283.150	-	-1.917200 00	4.000000-03
3	293.150	-	-1.637600 00	4.000000-03
4	303.150	-	-1.378800 00	4.000000-03
5	313.150	-	-1.139000 00	4.000000-03
6	323.150	-	-9.161000-01	4.000000-03
7	333.150	-	-7.085000-01	4.000000-03
8	343.150	-	-5.150000-01	4.000000-03
9	353.150	-	-3.341000-01	4.000000-03
10	363.150	-	-1.649000-01	4.000000-03
11	373.150	-	-6.300000-03	4.000000-03
12	383.150	-	1.424000-01	5.000000-03
13	393.150	-	2.822000-01	6.000000-03
14	403.150	-	4.138000-01	7.000000-03
15	413.150	-	5.376000-01	8.000000-03
16	423.150	-	6.544000-01	9.000000-03
17	433.150	-	7.647000-01	1.000000-02
18	443.150	-	8.689000-01	1.100000-02
19	453.150	-	9.674000-01	1.200000-02
20	463.150	-	1.060600 00	1.200000-02
21	473.150	-	1.148900 00	1.300000-02
22	483.150	-	1.232700 00	1.400000-02
23	493.150	-	1.312200 00	1.500000-02
24	503.150	-	1.388600 00	1.500000-02
25	513.150	-	1.459400 00	1.600000-02
26	523.150	-	1.527600 00	1.600000-02
27	533.150	-	1.586000 00	1.700000-02
28	543.150	-	1.654200 00	1.700000-02
29	553.150	-	1.713100 00	1.800000-02
30	563.150	-	1.768200 00	1.800000-02
31	573.150	-	1.822700 00	1.900000-02
32	583.150	-	1.873800 00	1.900000-02
33	593.150	-	1.922700 00	1.900000-02
34	603.150	-	1.969400 00	2.000000-02

35	613.150	-	2.014900 00	2.000000-02
36	623.150	-	2.057000 00	2.000000-02

****

2 H2O (L), H(T)-H(273.16) OSBORNE, STIMSON, AND GINNINGS, 1939

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 73
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
H2O (L)	1.000	NO	0
H2O (L)	-1.000	NO	0

INDEX	TEMPERATURE T2	TEMPERATURE T1	HT2-HT1	ERROR
37	278.150	273.160	9.053720 01	4.526860-02
38	283.150	273.160	1.807860 02	9.039310-02
39	288.150	273.160	2.708730 02	1.354370-01
40	293.150	273.160	3.608520 02	1.804260-01
41	298.150	273.160	4.507590 02	2.253800-01
42	303.150	273.160	5.406300 02	2.703150-01
43	308.150	273.160	6.305010 02	3.152510-01
44	313.150	273.160	7.203720 02	3.601860-01
45	318.150	273.160	8.102430 02	4.051210-01
46	323.150	273.160	9.001500 02	4.500750-01
47	328.150	273.160	9.900750 02	4.950370-01
48	333.150	273.160	1.080060 03	5.400270-01
49	338.150	273.160	1.170090 03	5.850430-01
50	343.150	273.160	1.260180 03	6.300870-01
51	348.150	273.160	1.350330 03	6.751660-01
52	353.150	273.160	1.440560 03	7.202820-01
53	358.150	273.160	1.530890 03	7.654430-01
54	363.150	273.160	1.621300 03	8.106480-01
55	368.150	273.160	1.711830 03	8.559170-01
56	373.150	273.160	1.802500 03	9.012480-01
57	378.150	273.160	1.893210 03	9.466070-01
58	383.150	273.160	1.984150 03	9.920740-01
59	388.150	273.160	2.075260 03	1.037630 00
60	393.150	273.160	2.166550 03	1.083280 00
61	398.150	273.160	2.258030 03	1.129010 00
62	403.150	273.160	2.349680 03	1.174840 00
63	408.150	273.160	2.441690 03	1.220850 00
64	413.150	273.160	2.533890 03	1.266940 00
65	418.150	273.160	2.626260 03	1.313130 00
66	423.150	273.160	2.719000 03	1.359500 00
67	428.150	273.160	2.811910 03	1.405960 00
68	433.150	273.160	2.905180 03	1.452590 00
69	438.150	273.160	2.999000 03	1.499500 00
70	443.150	273.160	3.092990 03	1.546500 00
71	448.150	273.160	3.187350 03	1.593670 00
72	453.150	273.160	3.282240 03	1.641120 00
73	458.150	273.160	3.377500 03	1.688750 00
74	463.150	273.160	3.473110 03	1.736560 00
75	468.150	273.160	3.569450 03	1.784720 00
76	473.150	273.160	3.665960 03	1.833980 00

77	478.150	273.160	3.76338D 03	1.88169D 00
78	483.150	273.160	3.861160 03	1.93058D 00
79	488.150	273.160	3.959650 03	1.97983D 00
80	493.150	273.160	4.058690 03	2.029340 00
81	498.150	273.160	4.158620 03	2.079310 00
82	503.150	273.160	4.259100 03	2.129550 00
83	508.150	273.160	4.360480 03	2.180240 00
84	513.150	273.160	4.462760 03	2.231380 00
85	518.150	273.160	4.565930 03	2.282970 00
86	523.150	273.160	4.670010 03	2.335010 00
87	528.150	273.160	4.775170 03	2.387590 00
88	533.150	273.160	4.881410 03	2.440700 00
89	538.150	273.160	4.988910 03	2.494450 00
90	543.150	273.160	5.097490 03	2.548740 00
91	548.150	273.160	5.207690 03	2.603840 00
92	553.150	273.160	5.319330 03	2.659660 00
93	558.150	273.160	5.432590 03	2.716300 00
94	563.150	273.160	5.547830 03	2.773920 00
95	568.150	273.160	5.664880 03	2.832440 00
96	573.150	273.160	5.784080 03	2.892040 00
97	578.150	273.160	5.905800 03	2.952900 00
98	583.150	273.160	6.030230 03	3.015120 00
99	588.150	273.160	6.157720 03	3.078860 00
100	593.150	273.160	6.288620 03	3.144310 00
101	598.150	273.160	6.423490 03	3.211750 00
102	603.150	273.160	6.563050 03	3.281520 00
103	608.150	273.160	6.708180 03	3.354090 00
104	613.150	273.160	6.859250 03	3.429630 00
105	618.150	273.160	7.018250 03	3.509130 00
106	623.150	273.160	7.187690 03	3.593850 00
107	628.150	273.160	7.371180 03	3.685590 00
108	633.150	273.160	7.576100 03	3.788050 00
109	638.150	273.160	7.817030 03	3.908510 00

****

3 H+ + OH- = H2O(L), DELTA CP, REACTION. ACKERMANN, 1958.

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 4
THE TYPE OF DATA IS: HEAT CAP

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
H2O (L)	1.000	NO	0
H+	-1.000	NO	0
OH-	-1.000	NO	0

INDEX	TEMPERATURE T2	TEMPERATURE T1	HEAT CAP	ERROR
110	283.150	-	6.92000D 01	3.00000D 00
111	303.150	-	5.01000D 01	3.00000D 00
112	323.150	-	4.18000D 01	3.00000D 00
113	343.150	-	4.23000D 01	3.00000D 00

****

4 H2O = OH- + H+, HEAT OF IONIZATION. OLOFSSON AND OLOFSSON, 1973.

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 6
THE TYPE OF DATA IS: ENTHALPY

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
H2O (L)	-1.000	NO	0
H+	1.000	NO	0
OH-	1.000	NO	0

INDEX	TEMPERATURE T2	T1	ENTHALPY	ERROR
114	298.150	-	1.336520 04	4.780110 00
115	323.150	-	1.217020 04	4.780110 00
116	347.550	-	1.115440 04	4.780110 00
117	373.550	-	1.005500 04	4.780110 00
118	398.450	-	8.926860 03	4.780110 00
119	417.750	-	7.994740 03	4.780110 00

****

5 LOG KW BIGNOLD, BREWER, AND HEARN, 1971.

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 24
THE TYPE OF DATA IS: LOG K

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
H2O (L)	-1.000	NO	0
H+	1.000	NO	0
OH-	1.000	NO	0

INDEX	TEMPERATURE T2	T1	LOG K	ERROR
120	324.150	-	-1.324100 01	2.100000-02
121	334.050	-	-1.299150 01	2.100000-02
122	343.650	-	-1.280160 01	1.300000-02
123	353.350	-	-1.264170 01	1.000000-02
124	363.050	-	-1.249000 01	2.800000-02
125	372.450	-	-1.223430 01	3.900000-02
126	381.750	-	-1.207450 01	2.500000-02
127	391.150	-	-1.198640 01	1.400000-02
128	400.450	-	-1.186990 01	1.400000-02
129	409.850	-	-1.176720 01	2.000000-02
130	419.150	-	-1.172080 01	2.400000-02
131	428.550	-	-1.160760 01	1.700000-02
132	437.850	-	-1.154770 01	1.500000-02
133	447.350	-	-1.147280 01	8.000000-03
134	456.750	-	-1.139290 01	8.000000-03
135	466.150	-	-1.133260 01	1.400000-02
136	475.650	-	-1.127900 01	8.000000-03
137	485.250	-	-1.125860 01	8.000000-03
138	494.850	-	-1.122830 01	8.000000-03

139	504.550	-	-1.121550 01	8.000000-03
140	514.350	-	-1.120210 01	8.000000-03
141	524.150	-	-1.119560 01	9.000000-03
142	534.150	-	-1.120380 01	9.000000-03
143	544.150	-	-1.121970 01	1.700000-02

****

6 H2O = OH- + H+, LOG Kw. SWEFTON, MESMER & BAES, PERS COMM, 1973.

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 7
THE TYPE OF DATA IS: LOG K

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
H2O (L)	-1.000	NO	0
H+	1.000	NO	0
OH-	1.000	NO	0

INDEX	TEMPERATURE T2	T1	LOG K	ERROR
144	273.150	-	-1.494100 01	9.000000-03
145	323.150	-	-1.327200 01	6.000000-03
146	373.150	-	-1.226400 01	9.000000-03
147	423.150	-	-1.164200 01	1.200000-02
148	473.150	-	-1.130200 01	1.200000-02
149	523.150	-	-1.119600 01	1.500000-02
150	573.150	-	-1.130100 01	4.500000-02

THE INDEX OF THE LAST ITEM OF THE ABOVE DATA SETS IN THE VECTORS X(1,I), YO(I), AND SIGYO(I) IS AS FOLLOWS:

DATA SET	INDEX
1	36
2	105
3	113
4	115
5	143
6	150

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

NUMBER OF CYCLES IN THIS JOB IS 3

NUMBER OF PARAMETERS TO BE VARIED IS 11

NUMBER OF INDEPENDENT VARIABLES PER OBSERVATION IS 2

DERIVATIVES PROGRAMMED IN SUBROUTINE EAFH2O.

WEIGHTS TO BE SUPPLIED BY USER

NUMBER OF PARAMETERS READ IS 28

NUMBER OF OBSERVATIONS READ IS 150

TRIAL CONSTANTS

I	P(I)	KI(I)
	H2O (G)	
1	1.7610D 00	0
2	3.2926D-03	0
3	-5.3334D 04	0
4	-4.5160D 04	0
5	4.2886D 01	0
6	-1.1500D-06	0
7	8.6459D 01	0
	H2O (L)	
8	2.3564D 01	1
9	-1.7286D-02	1
10	0.0	0
11	-5.7692D 04	1
12	-1.0972D 02	1
13	5.2422D-05	1
14	-1.0696D 03	1
	H+	
15	0.0	0
16	0.0	0
17	0.0	0
18	0.0	0
19	0.0	0
20	0.0	0
21	0.0	0
	OH-	
22	3.0806D 02	1
23	-3.0582D-01	1
24	-1.3986D 07	1
25	-1.4962D 05	1
26	-1.6526D 03	1
27	0.0	0
28	0.0	0

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 1

INDEX	T(2)	T(1)	Y(OBS)	Y(CALC)	OBS-CALC	SIG(O)	(O-C)/SIG(O)
H2O(L) = H2O(G),LOG K.			HAAS, 1970				
1	273.160		-2.2197	-2.2262	0.0065	0.0080	0.8126
2	283.150		-1.9172	-1.9229	0.0057	0.0040	1.4170
3	293.150		-1.6376	-1.6426	0.0050	0.0040	1.2461
4	303.150		-1.3788	-1.3833	0.0045	0.0040	1.1135
5	313.150		-1.1390	-1.1428	0.0038	0.0040	0.9453
6	323.150		-0.9161	-0.9193	0.0032	0.0040	0.8056
7	333.150		-0.7085	-0.7113	0.0028	0.0040	0.7059
8	343.150		-0.5150	-0.5173	0.0023	0.0040	0.5819
9	353.150		-0.3341	-0.3361	0.0020	0.0040	0.5014
10	363.150		-0.1649	-0.1666	0.0017	0.0040	0.4142
11	373.150		-0.0063	-0.0077	0.0014	0.0040	0.3562
12	383.150		0.1424	0.1413	0.0011	0.0050	0.2127
13	393.150		0.2822	0.2813	0.0009	0.0060	0.1441
14	403.150		0.4138	0.4130	0.0008	0.0070	0.1148
15	413.150		0.5376	0.5370	0.0006	0.0080	0.0812
16	423.150		0.6544	0.6538	0.0006	0.0090	0.0707
17	433.150		0.7647	0.7639	0.0008	0.0100	0.0751
18	443.150		0.8689	0.8680	0.0009	0.0110	0.0846
19	453.150		0.9674	0.9662	0.0012	0.0120	0.0960
20	463.150		1.0606	1.0592	0.0014	0.0130	0.1157
21	473.150		1.1489	1.1471	0.0018	0.0130	0.1410
22	483.150		1.2327	1.2303	0.0024	0.0140	0.1735
23	493.150		1.3122	1.3091	0.0031	0.0150	0.2089
24	503.150		1.3886	1.3837	0.0049	0.0150	0.3254
25	513.150		1.4594	1.4545	0.0049	0.0160	0.3085
26	523.150		1.5276	1.5215	0.0061	0.0160	0.3796
27	533.150		1.5860	1.5851	0.0009	0.0170	0.0535
28	543.150		1.6542	1.6454	0.0088	0.0170	0.5205
29	553.150		1.7131	1.7025	0.0106	0.0180	0.5908
30	563.150		1.7682	1.7566	0.0116	0.0180	0.6457
31	573.150		1.8227	1.8078	0.0149	0.0190	0.7837
32	583.150		1.8738	1.8563	0.0175	0.0190	0.9224
33	593.150		1.9227	1.9021	0.0206	0.0190	1.0868
34	603.150		1.9694	1.9452	0.0242	0.0200	1.2099
35	613.150		2.0149	1.9858	0.0291	0.0200	1.4573
36	623.150		2.0570	2.0237	0.0333	0.0200	1.6652
H2O (L), H(T)-H(273.16)			OSBORNE, STIMSON, AND GINNINGS, 1939				
37	278.150	273.160	90.5372	90.2942	0.2430	0.0453	5.3677
38	283.150	273.160	180.7863	180.6498	0.1364	0.0904	1.5093
39	288.150	273.160	270.9730	270.8554	-0.0262	0.1354	-0.1938
40	293.150	273.160	360.8521	361.0569	-0.2047	0.1804	-1.1347
41	298.150	273.160	450.7590	451.1360	-0.3768	0.2254	-1.6718
42	303.150	273.160	540.6301	541.1501	-0.5202	0.2703	-1.9243
43	308.150	273.160	630.5010	631.1138	-0.6127	0.3153	-1.9435
44	313.150	273.160	720.3718	721.0400	-0.6682	0.3602	-1.8552
45	318.150	273.160	810.2429	810.9436	-0.7007	0.4051	-1.7295
46	323.150	273.160	900.1499	900.8379	-0.6880	0.4501	-1.5285
47	328.150	273.160	990.0747	990.7368	-0.6621	0.4950	-1.3375
48	333.150	273.160	1080.0537	1080.6550	-0.6012	0.5400	-1.1132
49	338.150	273.160	1170.0867	1170.6060	-0.5192	0.5850	-0.8875
50	343.150	273.160	1260.1738	1260.6042	-0.4305	0.6301	-0.6833

51	348.150	273.160	1350.3328	1350.6641	-0.3313	0.6752	-0.4907
52	353.150	273.160	1440.5640	1440.7998	-0.2359	0.7203	-0.3275
53	358.150	273.160	1530.8850	1531.0256	-0.1407	0.7654	-0.1838
54	363.150	273.160	1621.2961	1621.3564	-0.0604	0.8106	-0.0745
55	368.150	273.160	1711.8333	1711.8069	0.0265	0.8559	0.0309
56	373.150	273.160	1802.4966	1802.3914	0.1051	0.9012	0.1166
57	378.150	273.160	1893.2139	1893.1252	0.0885	0.9466	0.0935
58	383.150	273.160	1984.1472	1984.0234	0.1237	0.9921	0.1247
59	388.150	273.160	2075.2605	2075.1013	0.1593	1.0376	0.1535
60	393.150	273.160	2166.5540	2166.3740	0.1799	1.0833	0.1661
61	398.150	273.160	2258.0276	2257.8577	0.1697	1.1290	0.1503
62	403.150	273.160	2349.6812	2349.5681	0.1129	1.1748	0.0961
63	408.150	273.160	2441.6948	2441.5217	0.1731	1.2208	0.1418
64	413.150	273.160	2533.8887	2533.7349	0.1538	1.2669	0.1214
65	418.150	273.160	2626.2625	2626.2246	0.0380	1.3131	0.0289
66	423.150	273.160	2718.9066	2719.0081	-0.0116	1.3595	-0.0086
67	428.150	273.160	2811.9106	2812.1035	-0.1930	1.4060	-0.1373
68	433.150	273.160	2905.1848	2905.5291	-0.3444	1.4526	-0.2371
69	438.150	273.160	2998.9990	2999.3040	-0.3048	1.4995	-0.2033
70	443.150	273.160	3092.9937	3093.4475	-0.4539	1.5465	-0.2935
71	448.150	273.160	3187.3481	3187.9805	-0.6323	1.5937	-0.3968
72	453.150	273.160	3282.2429	3282.9241	-0.6812	1.6411	-0.4151
73	458.150	273.160	3377.4978	3378.3008	-0.8029	1.6887	-0.4755
74	463.150	273.160	3473.1128	3474.1340	-1.0212	1.7366	-0.5881
75	468.150	273.160	3569.4482	3570.4490	-1.0007	1.7847	-0.5607
76	473.150	273.160	3665.9636	3667.2717	-1.3081	1.8330	-0.7136
77	478.150	273.160	3763.3794	3764.6304	-1.2512	1.8817	-0.6649
78	483.150	273.160	3861.1550	3862.5554	-1.4003	1.9306	-0.7253
79	488.150	273.160	3959.6511	3961.0791	-1.4278	1.9798	-0.7212
80	493.150	273.160	4058.6875	4060.2363	-1.5489	2.0293	-0.7633
81	498.150	273.160	4158.6211	4160.0625	-1.4415	2.0793	-0.6933
82	503.150	273.160	4259.0977	4260.6055	-1.5074	2.1295	-0.7079
83	508.150	273.160	4360.4766	4361.9102	-1.4323	2.1802	-0.6569
84	513.150	273.160	4462.7539	4464.0195	-1.2656	2.2314	-0.5676
85	518.150	273.160	4565.9297	4566.9961	-1.0662	2.2830	-0.4670
86	523.150	273.160	4670.0078	4670.9023	-0.8936	2.3350	-0.3827
87	528.150	273.160	4775.1680	4775.8086	-0.6385	2.3876	-0.2674
88	533.150	273.160	4881.4063	4881.7852	-0.3795	2.4407	-0.1555
89	538.150	273.160	4988.9063	4988.9326	-0.0254	2.4945	-0.0102
90	543.150	273.160	5097.4883	5097.3438	0.1427	2.5487	0.0560
91	548.150	273.160	5207.6875	5207.1367	0.5497	2.6038	0.2111
92	553.150	273.160	5319.3281	5318.4453	0.8834	2.6597	0.3321
93	558.150	273.160	5432.5898	5431.4180	1.1713	2.7163	0.4312
94	563.150	273.160	5547.8320	5546.2344	1.5971	2.7739	0.5758
95	568.150	273.160	5664.8750	5663.0977	1.7753	2.8324	0.6268
96	573.150	273.160	5784.0781	5782.2539	1.8257	2.8920	0.6313
97	578.150	273.160	5905.8008	5903.9766	1.8262	2.9529	0.6184
98	583.150	273.160	6030.2266	6028.6055	1.6235	3.0151	0.5385
99	588.150	273.160	6157.7148	6156.5352	1.1818	3.0789	0.3839
100	593.150	273.160	6288.6211	6288.2344	0.3890	3.1443	0.1237
101	598.150	273.160	6423.4922	6424.2734	-0.7816	3.2117	-0.2434
102	603.150	273.160	6563.0430	6565.3359	-2.2929	3.2815	-0.6990
103	608.150	273.160	6708.1758	6712.2539	-4.0777	3.3541	-1.2157
104	613.150	273.160	6859.2539	6866.0391	-6.7867	3.4296	-1.9788
105	618.150	273.160	7018.2500	7027.9375	-9.6860	3.5091	-2.7602
106	623.150	273.160	7187.6914	7199.4883	-11.7958	3.5938	-3.2822
107	628.150	273.160	7371.1797	7382.6133	-11.4339	3.6856	-3.1023
108	633.150	273.160	7576.0938	7579.7188	-3.6250	3.7880	-0.9570
109	638.150	273.160	7817.0234	7793.8516	23.1736	3.9085	5.9290

H+ + OH- = H2O(L), DELTA CP, REACTION. ACKERMANN, 1958.

110	283.150	69.2000	57.6360	11.5640	3.0000	3.8547
111	303.150	50.1000	47.5468	2.5532	3.0000	0.8511
112	323.150	41.8000	41.5055	0.2945	3.0000	0.0982
113	343.150	42.3000	38.6071	3.6929	3.0000	1.2310

H2C = CH- + H+, HEAT OF IONIZATION — OLOFSSON AND OLOFSSON, 1973.

114	298.150	13265.1953	13486.3008	-121.1052	4.7801	-25.3152
115	323.150	12170.1680	12358.8047	-188.6371	4.7801	-39.4629
116	347.550	11154.3745	11393.1055	-238.7103	4.7801	-49.9382
117	373.550	10054.9688	10398.2070	-343.2375	4.7801	-71.8059
118	398.450	8926.8594	9396.6836	-469.8237	4.7801	-98.2872
119	417.750	7994.7383	8547.6211	-552.8833	4.7801	-115.6632

LOG KW — BIGNOLO, BREWER, AND HEARN, 1971.

120	324.150	-13.2410	-13.0027	-0.2383	0.0210	-11.3469
121	334.050	-12.9919	-12.7606	-0.2313	0.0210	-11.0354
122	343.650	-12.8016	-12.5462	-0.2554	0.0130	-19.6485
123	353.350	-12.6417	-12.3479	-0.2938	0.0130	-29.3933
124	363.050	-12.4900	-12.1663	-0.3237	0.0280	-11.5614
125	372.450	-12.2343	-12.0049	-0.2294	0.0390	-5.8826
126	381.750	-12.0745	-11.8582	-0.2163	0.0250	-8.6521
127	391.150	-11.9864	-11.7221	-0.2643	0.0140	-18.8771
128	400.450	-11.8699	-11.5987	-0.2712	0.0140	-19.3686
129	409.850	-11.7672	-11.4847	-0.2825	0.0200	-14.1256
130	419.150	-11.7208	-11.3818	-0.3390	0.0240	-14.1254
131	428.550	-11.6076	-11.2873	-0.3203	0.0170	-18.8415
132	437.850	-11.5477	-11.2027	-0.3450	0.0150	-22.9969
133	447.350	-11.4728	-11.1251	-0.3477	0.0080	-43.4573
134	456.750	-11.3929	-11.0567	-0.3362	0.0080	-42.0352
135	466.150	-11.3326	-10.9962	-0.3364	0.0140	-24.0267
136	475.650	-11.2790	-10.9429	-0.3361	0.0080	-42.0110
137	485.250	-11.2586	-10.8967	-0.3619	0.0080	-45.2341
138	494.850	-11.2283	-10.8580	-0.3703	0.0080	-46.2845
139	504.550	-11.2155	-10.8263	-0.3892	0.0080	-48.6516
140	514.350	-11.2021	-10.8015	-0.4006	0.0080	-50.0710
141	524.150	-11.1956	-10.7839	-0.4117	0.0090	-45.7413
142	534.150	-11.2038	-10.7732	-0.4306	0.0090	-47.8459
143	544.150	-11.2197	-10.7695	-0.4502	0.0170	-26.4845

H2C = CH- + H+, LOG KW. — SWEETON, MESMER & BAES, PERS COMM, 1973.

144	273.150	-14.9410	-14.7126	-0.2284	0.0090	-25.3772
145	323.150	-13.2720	-13.0285	-0.2435	0.0060	-40.5905
146	373.150	-12.2640	-11.9934	-0.2706	0.0090	-30.0664
147	423.150	-11.6420	-11.3404	-0.3016	0.0120	-25.1300
148	473.150	-11.3020	-10.9562	-0.3458	0.0120	-28.8169
149	523.150	-11.1960	-10.7854	-0.4106	0.0150	-27.3732
150	573.150	-11.3010	-10.7975	-0.5035	0.0450	-11.1883

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 0.6250 05

SQRTF(SUM(W*(O-C)**2)/(NC-NV)) IS 0.2120D 02

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
H2O (G)						
1	1.76055830430D 00	1.76055830430 C0				
2	3.28246628230-03	3.28246628230-C3				
3	-5.33383252400 04	-5.33383252400 C4				
4	-4.5159e3e4e10 04	-4.5159E36461D C4				
5	4.28795457410 01	4.28795457410 C1				
6	-1.1500151250D-06	-1.1500151250D-C6				
7	8.6459029383D 01	8.6459C29383D C1				
H2O (L)						
8	2.3567900000D 01	-2.8925C550320-03	2.35650074940 01	9.5732249978C-02	-1.2274579178D-02	0.4062
9	-1.7282600000D-02	-3.2779924886D-C7	-1.7282927799C-02	2.6700530110C-04	1.8966650365D-03	1.5449
10	0.C	0.0				
11	-5.7691600000D 04	-5.4619609358D-C2	-5.7691654620C 04	1.8057794322C 01	9.4675012690-05	0.0313
12	-1.0971800000D 02	-1.2941082110D-C3	-1.0971929411D 02	4.2015647378C-01	1.1794718709D-03	0.3829
13	5.2422200000D-05	7.7626351701D-10	5.2422976264C-05	7.3233395706C-C7	1.4807656420-03	1.3970
14	-1.0695500000D 03	2.2421269441D-03	-1.0695473[illegible]3C 03	1.0096675710C 01	-2.0963317658C-04	0.9443
H+						
15	0.C	0.0				
16	0.0	0.0				
17	0.C	0.0				
18	0.C	0.0				
19	0.C	0.0				
20	0.0	0.0				
21	0.C	0.0				
OH-						
22	3.C805700000D 02	4.5117542967D C1	3.5317654297C 02	1.5375573C07C 01	1.2774784658D 01	4.3435
23	-3.C581700000D-01	-5.0892E274240-C2	-3.5670982742C-01	1.4317173800C-C2	1.4267295240 01	4.0137
24	-1.3586400000D 07	-1.5440117655D C6	-1.5530411765C 07	6.4429143835C 05	9.9418558050C 00	4.1486
25	-1.4982200000D 05	-1.4228195922D 04	-1.6404819592C 05	5.4693111194C 03	8.6731E036750 00	3.3340
26	-1.6525900000D 03	-2.3693568593D C2	-1.8895296859C 03	8.2676027217C 01	1.2539611719D 01	4.3755
27	0.C	0.0				
28	0.C	0.0				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

SUM(W*(O-C)**2) IS 0.2220 03

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.1262D 01

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 2

INDEX	T(2)	T(1)	Y(OBS)	Y(CALC)	OBS-CALC	SIG(Y)	(O-C)/SIG(C)
H2O(L) = H2O(G),LOG K.			HAAS, 1970				
1	273.160		-2.2197	-2.2230	0.0033	0.0080	0.4163
2	283.150		-1.9172	-1.9197	0.0025	0.0040	0.6180
3	293.150		-1.6376	-1.6394	0.0018	0.0040	0.4412
4	303.150		-1.3788	-1.3800	0.0012	0.0040	0.3028
5	313.150		-1.1390	-1.1395	0.0005	0.0040	0.1291
6	323.150		-0.9161	-0.9161	-0.0000	0.0040	-0.0120
7	333.150		-0.7085	-0.7080	-0.0005	0.0040	-0.1210
8	343.150		-0.5150	-0.5140	-0.0010	0.0040	-0.2501
9	353.150		-0.3341	-0.3328	-0.0013	0.0040	-0.3194
10	363.150		-0.1649	-0.1632	-0.0017	0.0040	-0.4274
11	373.150		-0.0063	-0.0043	-0.0020	0.0040	-0.4961
12	383.150		0.1424	0.1447	-0.0023	0.0050	-0.4679
13	393.150		0.2822	0.2848	-0.0026	0.0060	-0.4260
14	403.150		0.4138	0.4164	-0.0026	0.0070	-0.3764
15	413.150		0.5376	0.5404	-0.0028	0.0080	-0.3506
16	423.150		0.6544	0.6572	-0.0028	0.0090	-0.3149
17	433.150		0.7647	0.7674	-0.0027	0.0100	-0.2735
18	443.150		0.8689	0.8715	-0.0026	0.0110	-0.2338
19	453.150		0.9674	0.9698	-0.0024	0.0120	-0.1971
20	463.150		1.0606	1.0627	-0.0021	0.0120	-0.1747
21	473.150		1.1489	1.1506	-0.0017	0.0130	-0.1318
22	483.150		1.2327	1.2338	-0.0011	0.0140	-0.0809
23	493.150		1.3122	1.3126	-0.0004	0.0150	-0.0295
24	503.150		1.3886	1.3873	0.0013	0.0150	0.0862
25	513.150		1.4594	1.4581	0.0013	0.0160	0.0834
26	523.150		1.5276	1.5251	0.0025	0.0160	0.1540
27	533.150		1.5860	1.5887	-0.0027	0.0170	-0.1559
28	543.150		1.6542	1.6490	0.0052	0.0170	0.3064
29	553.150		1.7131	1.7061	0.0070	0.0180	0.3879
30	563.150		1.7682	1.7602	0.0080	0.0180	0.4422
31	573.150		1.8227	1.8115	0.0112	0.0190	0.5902
32	583.150		1.8738	1.8600	0.0138	0.0190	0.7283
33	593.150		1.9227	1.9058	0.0169	0.0190	0.8921
34	603.150		1.9694	1.9489	0.0205	0.0200	1.0244
35	613.150		2.0149	1.9895	0.0254	0.0200	1.2711
36	623.150		2.0570	2.0274	0.0296	0.0200	1.4785
H2O (L), H(T)-H(273.16)			OSBORNE, STIMSON, AND GINNINGS, 1939				
37	278.150	273.160	90.5372	90.2791	0.2580	0.0453	5.7000
38	283.150	273.160	180.7863	180.6197	0.1665	0.0904	1.8425
39	288.150	273.160	270.8730	270.8542	0.0190	0.1354	0.1400
40	293.150	273.160	360.8521	360.9966	-0.1444	0.1804	-0.8006
41	298.150	273.160	450.7590	451.0605	-0.3014	0.2254	-1.3373
42	303.150	273.160	540.6301	541.0598	-0.4297	0.2703	-1.5896
43	308.150	273.160	630.5010	631.0081	-0.5071	0.3153	-1.6086
44	313.150	273.160	720.3718	720.9194	-0.5475	0.3602	-1.5202
45	318.150	273.160	810.2429	810.8076	-0.5649	0.4051	-1.3943
46	323.150	273.160	900.1499	900.6868	-0.5370	0.4501	-1.1932
47	328.150	273.160	990.0747	990.5708	-0.4961	0.4950	-1.0021
48	333.150	273.160	1080.0537	1080.4736	-0.4200	0.5400	-0.7777
49	338.150	273.160	1170.0867	1170.4097	-0.3229	0.5850	-0.5520
50	343.150	273.160	1260.1738	1260.3928	-0.2191	0.6301	-0.3477

51	348.150	273.160	1350.3328	1350.4375	-0.1047	0.6752	-0.1551
52	353.150	273.160	1440.5640	1440.5581	0.0058	0.7203	0.0081
53	358.150	273.160	1530.8850	1530.7688	0.1161	0.7654	0.1517
54	363.150	273.160	1621.2961	1621.0845	0.2116	0.8106	0.2610
55	368.150	273.160	1711.8333	1711.5198	0.3136	0.8559	0.3664
56	373.150	273.160	1802.4966	1802.0891	0.4074	0.9012	0.4520
57	378.150	273.160	1893.2139	1892.8079	0.4059	0.9466	0.4288
58	383.150	273.160	1984.1472	1983.6909	0.4562	0.9921	0.4599
59	388.150	273.160	2075.2605	2074.7534	0.5070	1.0376	0.4886
60	393.150	273.160	2166.5540	2166.0112	0.5427	1.0833	0.5010
61	398.150	273.160	2258.0276	2257.4797	0.5477	1.1290	0.4852
62	403.150	273.160	2349.6812	2349.1750	0.5060	1.1748	0.4307
63	408.150	273.160	2441.6948	2441.1133	0.5814	1.2208	0.4763
64	413.150	273.160	2533.8887	2533.3113	0.5773	1.2669	0.4557
65	418.150	273.160	2626.2625	2625.7859	0.4766	1.3131	0.3630
66	423.150	273.160	2718.9966	2718.5544	0.4422	1.3595	0.3252
67	428.150	273.160	2811.9106	2811.6345	0.2760	1.4060	0.1963
68	433.150	273.160	2905.1848	2905.0449	0.1398	1.4526	0.0962
69	438.150	273.160	2998.9993	2998.8047	0.1945	1.4995	0.1297
70	443.150	273.160	3092.9937	3092.9331	0.0605	1.5465	0.0391
71	448.150	273.160	3187.3481	3187.4509	-0.1027	1.5937	-0.0645
72	453.150	273.160	3282.2429	3282.3794	-0.1364	1.6411	-0.0831
73	458.150	273.160	3377.4978	3377.7410	-0.2431	1.6887	-0.1439
74	463.150	273.160	3473.1128	3473.5591	-0.4462	1.7366	-0.2569
75	468.150	273.160	3569.4482	3569.8586	-0.4105	1.7847	-0.2300
76	473.150	273.160	3665.9636	3666.6663	-0.7028	1.8330	-0.3834
77	478.150	273.160	3763.3794	3764.0100	-0.6307	1.8817	-0.3352
78	483.150	273.160	3861.1550	3861.9199	-0.7647	1.9306	-0.3961
79	488.150	273.160	3959.6511	3960.4282	-0.7771	1.9798	-0.3925
80	493.150	273.160	4058.6875	4059.5706	-0.8830	2.0293	-0.4351
81	498.150	273.160	4158.6211	4159.3828	-0.7604	2.0793	-0.3657
82	503.150	273.160	4259.0977	4259.9102	-0.8112	2.1295	-0.3809
83	508.150	273.160	4360.4766	4361.1953	-0.7205	2.1802	-0.3307
84	513.150	273.160	4462.7539	4463.2930	-0.5401	2.2314	-0.2420
85	518.150	273.160	4565.9297	4566.2578	-0.3246	2.2830	-0.1422
86	523.150	273.160	4670.0078	4670.1484	-0.1369	2.3350	-0.0586
87	528.150	273.160	4775.1680	4775.0352	0.1333	2.3876	0.0558
88	533.150	273.160	4881.4063	4881.0000	0.4075	2.4407	0.1669
89	538.150	273.160	4988.9063	4988.1289	0.7767	2.4945	0.3114
90	543.150	273.160	5097.4883	5096.5273	0.9599	2.5487	0.3766
91	548.150	273.160	5207.6875	5206.3047	1.3820	2.6039	0.5308
92	553.150	273.160	5319.3281	5317.5977	1.7308	2.6597	0.6508
93	558.150	273.160	5432.5898	5430.5547	2.0339	2.7163	0.7488
94	563.150	273.160	5547.8320	5545.3555	2.4748	2.7739	0.8922
95	568.150	273.160	5664.8750	5662.2070	2.6680	2.8324	0.9420
96	573.150	273.160	5784.0781	5781.3438	2.7335	2.8920	0.9452
97	578.150	273.160	5905.8008	5903.0547	2.7492	2.9529	0.9310
98	583.150	273.160	6030.2266	6027.6680	2.5615	3.0151	0.8496
99	588.150	273.160	6157.7148	6156.5781	2.1350	3.0789	0.6934
100	593.150	273.160	6288.6211	6287.2656	1.3572	3.1443	0.4317
101	598.150	273.160	6423.4922	6423.2891	0.2017	3.2117	0.0628
102	603.150	273.160	6563.0430	6564.3398	-1.2955	3.2815	-0.3948
103	608.150	273.160	6708.1758	6711.2422	-3.0641	3.3541	-0.9136
104	613.150	273.160	6859.2539	6865.0117	-5.7580	3.4296	-1.6789
105	618.150	273.160	7018.2500	7026.8945	-8.6423	3.5091	-2.4628
106	623.150	273.160	7187.6914	7198.4297	-10.7369	3.5928	-2.9876
107	628.150	273.160	7371.1797	7381.5391	-10.3595	3.6856	-2.8109
108	633.150	273.160	7576.0938	7578.6289	-2.5358	3.7880	-0.6694
109	638.150	273.160	7817.0234	7792.7461	24.2779	3.9085	6.2116

H+ + OH- = H2O(L), DELTA CP, REACTION. ACKERMANN, 1958.

110	283.150	69.2000	60.5943	8.6057	3.0000	2.8686
111	303.150	50.1000	50.0836	0.0164	3.0000	0.0055
112	323.150	41.8000	44.0627	-2.2627	3.0000	-0.7542
113	343.150	42.3000	41.5267	0.7733	3.0000	0.2578

H2C = OH- + H+, HEAT OF IONIZATION — OLOFSSON AND OLOFSSON, 1973.

114	298.150	13365.1953	13365.4453	-0.2473	4.7801	-0.0517
115	323.150	12170.1680	12174.8320	-4.6628	4.7801	-0.9755
116	347.550	11154.3945	11141.7617	12.6304	4.7801	2.6423
117	373.550	10054.9688	10056.6172	-1.6454	4.7801	-0.3451
118	398.450	8926.8594	8941.5961	-15.1334	4.7801	-3.1659
119	417.750	7994.7383	7983.0352	11.7039	4.7801	2.4484

LOG KW — BIGNOLD, BREWER, AND HEARN, 1971.

120	324.150	-13.2410	-13.2560	0.0150	0.0210	0.7120
121	334.050	-12.9919	-13.0178	0.0259	0.0210	1.2331
122	343.650	-12.8016	-12.8075	0.0059	0.0130	0.4551
123	353.350	-12.6417	-12.6137	-0.0280	0.0100	-2.8047
124	363.050	-12.4900	-12.4368	-0.0532	0.0280	-1.9006
125	372.450	-12.2343	-12.2802	0.0459	0.0390	1.1778
126	381.750	-12.0745	-12.1386	0.0641	0.0250	2.5655
127	391.150	-11.9864	-12.0080	0.0216	0.0140	1.5440
128	400.450	-11.8699	-11.8904	0.0205	0.0140	1.4614
129	409.850	-11.7672	-11.7824	0.0152	0.0200	0.7625
130	419.150	-11.7208	-11.6860	-0.0348	0.0240	-1.4502
131	428.550	-11.6076	-11.5984	-0.0092	0.0170	-0.5410
132	437.850	-11.5477	-11.5211	-0.0266	0.0150	-1.7737
133	447.350	-11.4728	-11.4513	-0.0215	0.0080	-2.6846
134	456.750	-11.3929	-11.3911	-0.0018	0.0080	-0.2273
135	466.150	-11.3326	-11.3259	0.0067	0.0140	0.4768
136	475.650	-11.2790	-11.2952	0.0162	0.0080	2.0258
137	485.250	-11.2586	-11.2589	0.0003	0.0090	0.0343
138	494.850	-11.2283	-11.2306	0.0023	0.0080	0.2914
139	504.550	-11.2155	-11.2098	-0.0057	0.0080	-0.7166
140	514.350	-11.2021	-11.1968	-0.0053	0.0080	-0.6619
141	524.150	-11.1956	-11.1915	-0.0041	0.0090	-0.4561
142	534.150	-11.2038	-11.1939	-0.0099	0.0090	-1.1036
143	544.150	-11.2197	-11.2039	-0.0158	0.0170	-0.9265

H2C = CH- + H+, LOG KW. — SWEETON, MESMER & BAES, PERS COMM, 1973.

144	273.150	-14.9410	-14.9512	0.0102	0.0090	1.1282
145	323.150	-13.2720	-13.2813	0.0093	0.0060	1.5512
146	373.150	-12.2640	-12.2691	0.0051	0.0090	0.5658
147	423.150	-11.6420	-11.6475	0.0055	0.0120	0.4610
148	473.150	-11.3020	-11.3060	0.0040	0.0120	0.3342
149	523.150	-11.1960	-11.1917	-0.0043	0.0150	-0.2875
150	573.150	-11.3010	-11.2755	-0.0255	0.0450	-0.5669

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 2

SUM(W*(O-C)**2) IS 0.222E 03

SQRTF(SUM(W*(O-C)**2)/(NC-NV)) IS 0.12620 01

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

PARAMETERS AFTER LEAST SQUARES CYCLE 2

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
H2O (G)						
1	1.76095830430 00	1.76095830430 C0				
2	3.28246628230-03	3.28246628230-03				
3	-5.33383252400 04	-5.33383252400 C4				
4	-4.51598364610 04	-4.51598364610 C4				
5	4.28795457410 01	4.28795457410 01				
6	-1.15001512500-06	-1.15001512500-06				
7	8.64570293830 01	8.64590293830 C1				
H2O (L)						
8	2.35650074940 01	4.53460C05320-11	2.3565007495C 01	9.5732215363C-02	1.92429411840-10	0.4062
9	-1.72829277990-02	-1.28201C8607D-13	-1.72829277990-02	2.67CC520456C-04	7.41778751610-10	1.5449
10	C.C	0.0				
11	-5.76916546200 04	-5.21992702700-09	-5.76916546200 04	1.80577877930 01	9.04797593590-12	0.0013
12	-1.09769294110 02	-1.95984366560-10	-1.09719294110 02	4.20156321860-01	1.78623430650-10	0.3329
13	5.24229762640-05	3.47479647910-16	5.24229762640-05	7.32333652260-07	6.62838458770-13	1.3370
14	-1.06954775790 03	3.66834339450-09	-1.06954775790 03	1.00966720590 01	-3.42980794220-10	0.9440
H+						
15	C.C	0.0				
16	0.0	0.0				
17	C.C	0.0				
18	0.C	0.0				
19	C.C	0.0				
20	0.C	0.0				
21	0.C	0.0				
OH-						
22	3.53176542970 02	-6.74612468690-07	3.53176542290 02	1.52755674470 01	-1.91012818780-07	4.3535
23	-3.56709327420-01	6.26337197240-10	-3.56709826800-01	1.43171686230-02	-1.75587312200-07	4.0137
24	-1.55304117650 07	2.80157183320-02	-1.55304117370 07	6.44291205280 05	-1.80392630960-07	4.1486
25	-1.64048195920 05	2.40194080520-04	-1.64048195680 05	5.46930914180 03	-1.46416776800-07	3.3540
26	-1.88952960590 03	3.61790738590-06	-1.88952968230 03	8.26759973230 01	-1.91471317960-07	4.3755
27	C.C	0.0				
28	C.C	0.0				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 2

SUM(W*(O-C)**2) IS 0.2220 03

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.12620 01

SUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FOR REASON 1

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CORRELATION MATRIX

1	0.1000D 01	-0.9977D 00	-0.6163D 00	-0.5950D 00	0.9897D 00	0.7501D 00	-0.5789D-02	0.5387D-02	0.6090D-02	0.6023D-02
	0.5849D-02									
2	0.0	0.1000D 01	0.6122D 00	0.5917D 00	-0.9970D 00	-0.7863D 00	0.5865D-02	-0.5488D-02	-0.6113D-02	-0.6072D-02
	-0.5915D-02									
3	0.0	0.0	0.1000D 01	0.6908D 00	-0.6046D 00	-0.4475D 00	0.3516D-02	-0.3256D-02	-0.3731D-02	-0.1632D-02
	-0.3164D-02									
4	0.0	0.0	0.0	0.1000D 01	-0.9826D 00	-0.7357D 00	0.5740D-02	-0.5334D-02	-0.6051D-02	-0.5725D-02
	-0.5751D-02									
5	0.0	0.0	0.0	0.0	0.1000D 01	0.8169D 00	-0.5912D-02	0.5573D-02	0.6099D-02	0.6087D-02
	0.5961D-02									
6	0.0	0.0	0.0	0.0	0.0	0.1000D 01	-0.4817D-02	0.4732D-02	0.4676D-02	0.4753D-02
	0.4823D-02									
7	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01	-0.9992D 00	-0.9970D 00	-0.9992D 00
	-0.1000D 01									
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01	0.9933D 00	0.9977D 00
	0.9989D 00									
9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01	0.9992D 00
	0.9975D 00									
10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01
	0.9995D 00									
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.1000D 01									

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

TEMPERATURE T(2)	TEMPERATURE T(1)	LOG K OBSERVED	LOG K CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYO
H2O(L) = H2O(G), LOG K.			HAAS, 1970			
273.160	0.0	-2.2197D 00	-2.2230D 00	0.0033	0.1500	0.4163
283.150	0.0	-1.9172D 00	-1.9197D 00	0.0025	0.1289	0.6180
293.150	0.0	-1.6376D 00	-1.6394D 00	0.0018	0.1078	0.4412
303.150	0.0	-1.3768D 00	-1.3803D 00	0.0012	0.0878	0.3028
313.150	0.0	-1.1395D 00	-1.1395D 00	0.0005	0.0453	0.1291
323.150	0.0	-9.1610D-01	-9.1650D-01	-0.0000	-0.0052	-0.0120
333.150	0.0	-7.0859D-01	-7.0892D-01	-0.0005	-0.0683	-0.1210
343.150	0.0	-5.1500D-01	-5.1400D-01	-0.0010	-0.1943	-0.2501
353.150	0.0	-3.3410D-01	-3.3276D-01	-0.0013	-0.4016	-0.3354
363.150	0.0	-1.6490D-01	-1.6319D-01	-0.0017	-1.0368	-0.4274
373.150	0.0	-6.3000D-03	-4.3155D-03	-0.0020	-31.4995	-0.4961
383.150	0.0	1.4240D-01	1.4474D-01	-0.0023	-1.6429	-0.4679
393.150	0.0	2.8220D-01	2.8476D-01	-0.0026	-0.9057	-0.4260
403.150	0.0	4.1380D-01	4.1643D-01	-0.0026	-0.6367	-0.3764
413.150	0.0	5.3760D-01	5.4040D-01	-0.0028	-0.5217	-0.3506
423.150	0.0	6.5440D-01	6.5723D-01	-0.0028	-0.4331	-0.3149
433.150	0.0	7.6476D-01	7.6744D-01	-0.0027	-0.3577	-0.2735
443.150	0.0	8.6890D-01	8.7147D-01	-0.0026	-0.2960	-0.2338
453.150	0.0	9.6740D-01	9.6976D-01	-0.0024	-0.2445	-0.1971
463.150	0.0	1.0606D 00	1.0627D 00	-0.0021	-0.1976	-0.1747
473.150	0.0	1.1499D 00	1.1516D 00	-0.0017	-0.1491	-0.1319
483.150	0.0	1.2327D 00	1.2338D 00	-0.0011	-0.0919	-0.0809
493.150	0.0	1.3122D 00	1.3126D 00	-0.0004	-0.0337	-0.0295
503.150	0.0	1.3886D 00	1.3873D 00	0.0013	0.0931	0.0862
513.150	0.0	1.4594D 00	1.4581D 00	0.0013	0.0914	0.0834
523.150	0.0	1.5276D 00	1.5251D 00	0.0025	0.1613	0.1540
533.150	0.0	1.5886D 00	1.5887D 00	-0.0027	-0.1714	-0.1599
543.150	0.0	1.6542D 00	1.6490D 00	0.0052	0.3148	0.3064
553.150	0.0	1.7131D 00	1.7061D 00	0.0070	0.4076	0.3879
563.150	0.0	1.7682D 00	1.7602D 00	0.0080	0.4501	0.4422
573.150	0.0	1.8227D 00	1.8115D 00	0.0112	0.6152	0.5902
583.150	0.0	1.8738D 00	1.8600D 00	0.0138	0.7385	0.7283
593.150	0.0	1.9227D 00	1.9058D 00	0.0169	0.8815	0.8921
603.150	0.0	1.9694D 00	1.9489D 00	0.0205	1.0403	1.0243
613.150	0.0	2.0149D 00	1.9895D 00	0.0254	1.2617	1.2711
623.150	0.0	2.0570D 00	2.0274D 00	0.0296	1.4376	1.4785

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE ----- 0.0032 -0.8576 0.1248

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ---------- 0.0082 5.2143 0.4981

THE NUMBER OF OBSERVATIONS IS 36

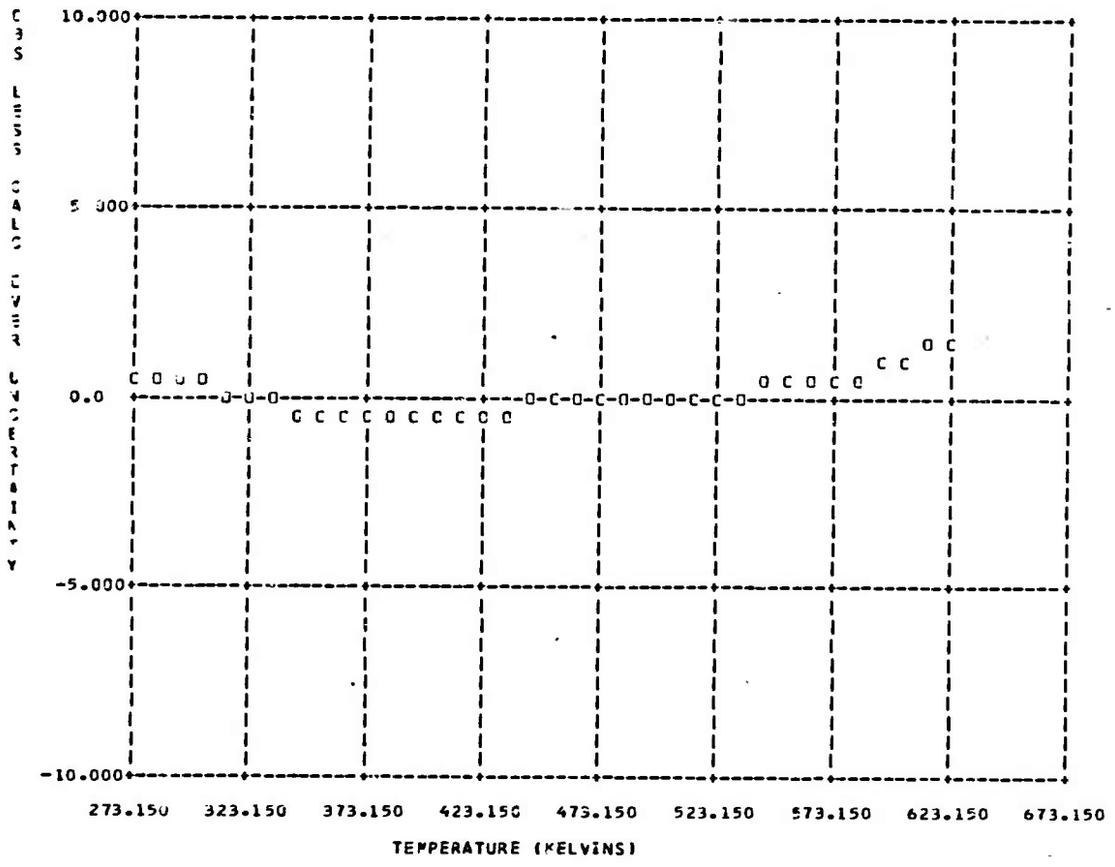
10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2O (G)	1.000	1.7609583D 00	3.2824663D-03	-5.33383250 04	-4.51598360 04	4.28795460 01	-1.15CC151D-06

		8.6459C29D C1					
H2C (L)	-1.000	2.35650070 C1 -1.0695478D C3	-1.7282928D-02	0.0	-5.76916559 04	-1.09719299 02	5.2422976D-05
		'A'/'G'	'B'	'C'	'D'	'E'	'F'
REACTION CONSTANTS		-2.18J4049D C1 1.1560068D C3	2.0565394D-02	-5.3338325D 04	1.2531818D 04	1.5259884D 02	-5.3572991D-05

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 12/31/73

H2O(L) = H2O(G),LOG K. HAAS, 1970



PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

TEMPERATURE		HT2-HT1		ERROR		
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT	OBS-CALC/SIGYD

H2O (L), H(T)-H(273.16) OSBORNE, STIMSON, AND GINNINGS, 1939

278.150	273.160	9.0537D 01	9.0279D 01	0.2590	0.2850	5.7000
283.150	273.160	1.8079D 02	1.8062D 02	0.1665	0.0921	1.8425
288.150	273.160	2.7087D 02	2.7085D 02	0.0190	0.0070	0.1400
293.150	273.160	3.6065D 02	3.6100D 02	-0.1444	-0.0400	-0.8006
298.150	273.160	4.5076D 02	4.5106D 02	-0.3014	-0.0669	-1.3373
303.150	273.160	5.4063D 02	5.4106D 02	-0.4297	-0.0795	-1.5896
308.150	273.160	6.3095D 02	6.3101D 02	-0.0071	-0.0804	-1.6086
313.150	273.160	7.2037D 02	7.2092D 02	-0.5475	-0.0760	-1.5202
318.150	273.160	8.1024D 02	8.1081D 02	-0.5649	-0.0697	-1.3943
323.150	273.160	9.0015D 02	9.0069D 02	-0.5370	-0.0597	-1.1932
328.150	273.160	9.9007D 02	9.9057D 02	-0.4961	-0.0501	-1.0021
333.150	273.160	1.0801D 03	1.0805D 03	-0.4280	-0.0389	-0.7777
338.150	273.160	1.1701D 03	1.1704D 03	-0.3229	-0.0276	-0.5520
343.150	273.160	1.2602D 03	1.2604D 03	-0.2191	-0.0174	-0.3477
348.150	273.160	1.3503D 03	1.3504D 03	-0.1047	-0.0078	-0.1551
353.150	273.160	1.4406D 03	1.4406D 03	0.0058	0.0004	0.0081
358.150	273.160	1.5309D 03	1.5308D 03	0.1161	0.0076	0.1517
363.150	273.160	1.6213D 03	1.6211D 03	0.2116	0.0130	0.2610
368.150	273.160	1.7118D 03	1.7115D 03	0.3136	0.0183	0.3664
373.150	273.160	1.8025D 03	1.8021D 03	0.4074	0.0226	0.4520
378.150	273.160	1.8932D 03	1.8928D 03	0.4059	0.0214	0.4288
383.150	273.160	1.9841D 03	1.9837D 03	0.4562	0.0230	0.4599
388.150	273.160	2.0753D 03	2.0748D 03	0.5070	0.0244	0.4886
393.150	273.160	2.1666D 03	2.1660D 03	0.5427	0.0251	0.5010
398.150	273.160	2.2580D 03	2.2575D 03	0.5477	0.0243	0.4852
403.150	273.160	2.3497D 03	2.3492D 03	0.5060	0.0215	0.4307
408.150	273.160	2.4417D 03	2.4411D 03	0.5814	0.0238	0.4763
413.150	273.160	2.5339D 03	2.5333D 03	0.5773	0.0228	0.4557
418.150	273.160	2.6263D 03	2.6258D 03	0.4766	0.0181	0.3630
423.150	273.160	2.7190D 03	2.7186D 03	0.4422	0.0163	0.3252
428.150	273.160	2.8119D 03	2.8116D 03	0.2760	0.0098	0.1963
433.150	273.160	2.9052D 03	2.9053D 03	-0.1397	-0.0048	-0.0962
438.150	273.160	2.9990D 03	2.9988D 03	0.1945	0.0065	0.1297
443.150	273.160	3.0932D 03	3.0929D 03	0.0605	0.0020	0.0391
448.150	273.160	3.1878D 03	3.1875D 03	-0.1027	-0.0032	-0.0645
453.150	273.160	3.2822D 03	3.2824D 03	-0.1364	-0.0042	-0.0831
458.150	273.160	3.3775D 03	3.3777D 03	-0.2431	-0.0072	-0.1439
463.150	273.160	3.4731D 03	3.4736D 03	-0.4462	-0.0128	-0.2569
468.150	273.160	3.5694D 03	3.5699D 03	-0.4105	-0.0115	-0.2300
473.150	273.160	3.6666D 03	3.6667D 03	-0.7028	-0.0192	-0.3834
478.150	273.160	3.7634D 03	3.7640D 03	-0.6307	-0.0168	-0.3352
483.150	273.160	3.8612D 03	3.8619D 03	-0.7647	-0.0198	-0.3961
488.150	273.160	3.9559D 03	3.9604D 03	-0.7771	-0.0196	-0.3925
493.150	273.160	4.0587D 03	4.0596D 03	-0.8830	-0.0218	-0.4351
498.150	273.160	4.1586D 03	4.1594D 03	-0.7604	-0.0183	-0.3657
503.150	273.160	4.2591D 03	4.2599D 03	-0.8112	-0.0190	-0.3809
508.150	273.160	4.3605D 03	4.3612D 03	-0.7209	-0.0165	-0.3307
513.150	273.160	4.4628D 03	4.4633D 03	-0.5401	-0.0121	-0.2420
518.150	273.160	4.5659D 03	4.5663D 03	-0.3246	-0.0071	-0.1422
523.150	273.160	4.6700D 03	4.6701D 03	-0.1369	-0.0029	-0.0586
528.150	273.160	4.7752D 03	4.7750D 03	0.1333	0.0028	0.0558

533.150	273.160	4.8814D 03	4.8810D 03	0.4075	0.0083	0.1669
538.150	273.160	4.9889D 03	4.9881D 03	0.7767	0.0156	0.3114
543.150	273.160	5.0975D 03	5.0965D 03	0.9599	0.0188	0.3766
548.150	273.160	5.2077D 03	5.2063D 03	1.3820	0.0265	0.5308
553.150	273.160	5.3193D 03	5.3176D 03	1.7308	0.0325	0.6508
558.150	273.160	5.4326D 03	5.4306D 03	2.0329	0.0374	0.7488
563.150	273.160	5.5478D 03	5.5454D 03	2.4748	0.0446	0.8922
568.150	273.160	5.6649D 03	5.6622D 03	2.6680	0.0471	0.9420
573.150	273.160	5.7841D 03	5.7813D 03	2.7335	0.0473	0.9452
578.150	273.160	5.9058D 03	5.9031D 03	2.7492	0.0466	0.9310
583.150	273.160	6.0302D 03	6.0277D 03	2.5615	0.0425	0.8496
588.150	273.160	6.1577D 03	6.1556D 03	2.1350	0.0347	0.6934
593.150	273.160	6.2886D 03	6.2873D 03	1.3572	0.0216	0.4317
598.150	273.160	6.4235D 03	6.4233D 03	0.2017	0.0031	0.0628
603.150	273.160	6.5630D 03	6.5643D 03	-1.2955	-0.0197	-0.3948
608.150	273.160	6.7082D 03	6.7112D 03	-3.0641	-0.0457	-0.9136
613.150	273.160	6.8593D 03	6.8650D 03	-5.7580	-0.0839	-1.6789
618.150	273.160	7.0183D 03	7.0269D 03	-8.6423	-0.1231	-2.4628
623.150	273.160	7.1877D 03	7.1984D 03	-10.7369	-0.1494	-2.9876
628.150	273.160	7.3712D 03	7.3815D 03	-10.3599	-0.1405	-2.8109
633.150	273.160	7.5761D 03	7.5786D 03	-2.5358	-0.0335	-0.6694
638.150	273.160	7.8170D 03	7.7927D 03	24.2779	0.3106	6.2116

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE ----- 0.0057 0.0001 0.0022

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ---------- 3.7013 0.0660 1.3197

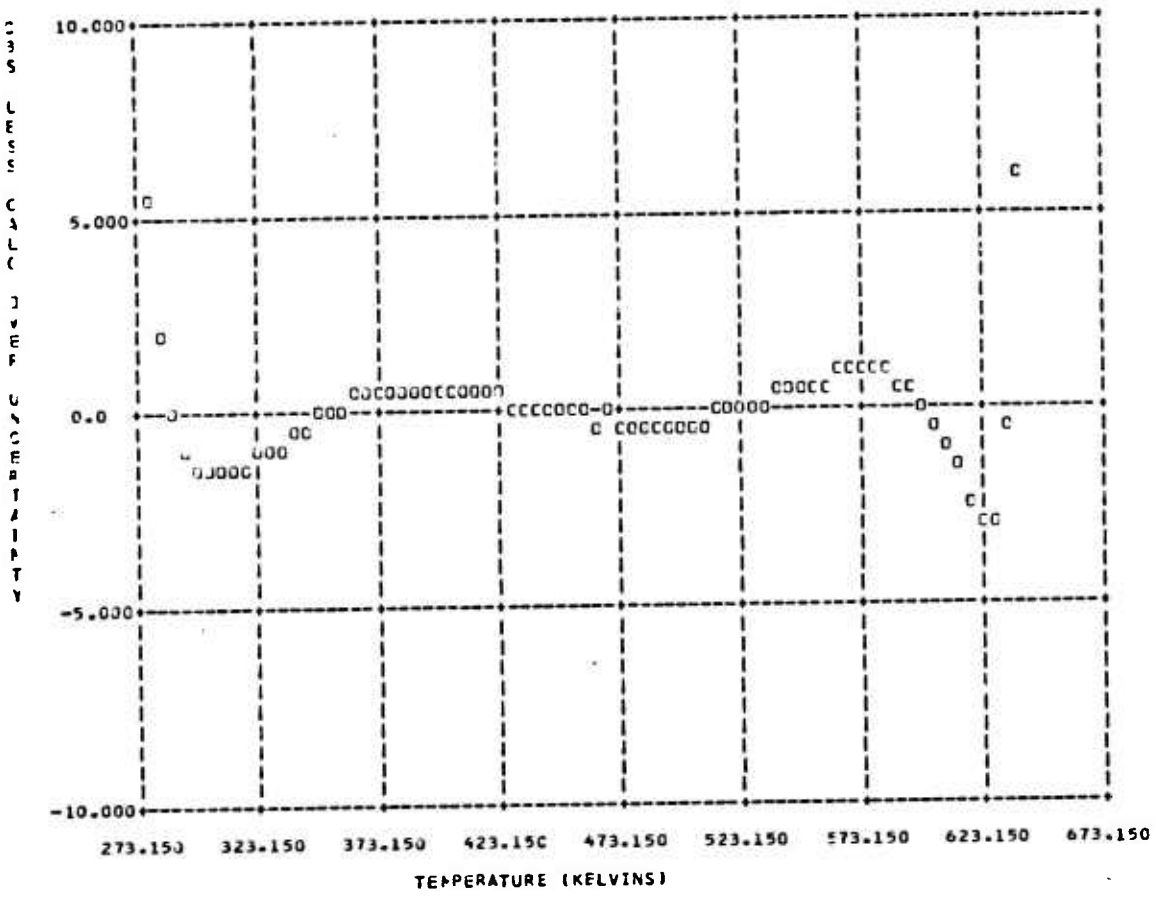
THE NUMBER OF OBSERVATIONS IS 73

10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2C (L)	1.000	2.3565007D 01 -1.0695478D 03	-1.7282928D-02	0.0	-5.7691655D 04	-1.0971929D 02	5.2422976D-05
H2C (L)	-1.000	2.3565007D 01 -1.0695478D 03	-1.7282928D-02	0.0	-5.7691655D 04	-1.0971929D 02	5.2422976D-05

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

H2O (L), P(T)=H(273.16) OSBORNE, STIMSON, AND GINNINGS, 1939



PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

TEMPERATURE T(2)	TEMPERATURE T(1)	HEAT CAP OBSERVED	HEAT CAP CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYD
H+ + OH- = H2O(L), DELTA CP, REACTION, ACKERMANN, 1958.						
283.150	0.0	6.92C0C D1	6.0594D 01	8.6057	12.436C	2.8686
303.150	0.0	5.01CGD D1	5.0084D 01	0.C164	0.0328	0.0055
323.150	0.0	4.18C0C D1	4.4063D 01	-2.2627	-5.4131	-0.7542
343.150	0.0	4.23CGD 01	4.1527D 01	0.7733	1.8282	0.2578
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				1.7832	2.2210	0.5944
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				4.0944	6.4724	1.3648
THE NUMBER OF OBSERVATIONS IS 4						

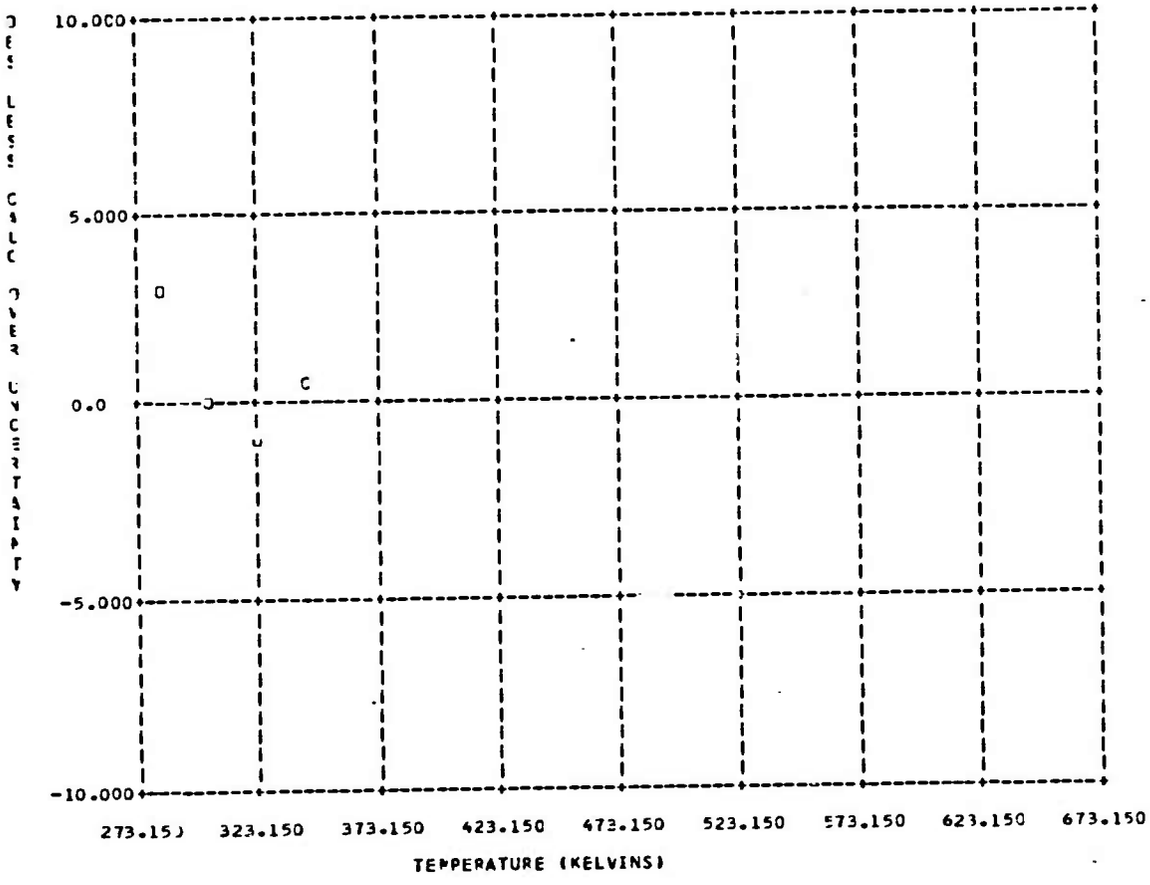
10/31/73----------

PHASE	CHARGE	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2O (L)	1.000	2.3565D07D C1 -1.0695478D C3	-1.7282928D-02	0.0	-5.7691655D 04	-1.0971929D 02	5.2422976D-05
H+	-1.000	0.0 0.0	0.0	D.C	D.C	D.D	C.0
OH-	-1.000	3.5317654D C2 0.0	-3.5670983D-01	-1.5530412D D7	-1.6404820D 05	-1.8895297D 03	0.C
		'A'/'G'	'B'/'G(IDN)'	'C'	'D'	'E'	'F'
REACTION CONSTANTS		-3.2961153D C2 -1.0695478D C3	3.3942690D-01 1.5530412D D7	D.0	1.D635654D D5	1.7798104D 03	5.2422976D-05

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

10/31/73

H+ + OH- = H2O(L), DELTA CP, REACTION. ACKERMANN, 1958.



PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

TEMPERATURE T(2)	TEMPERATURE T(1)	ENTHALPY OBSERVED	ENTHALPY CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYO
H2O = OH- + H+, HEAT OF IONIZATION		OLOFSSON AND OLOFSSON, 1973.				
298.150	0.0	1.33650 04	1.33650 04	-0.2473	-0.0019	-0.0517
323.150	0.0	1.21700 04	1.2175D 04	-4.6628	-0.0383	-0.9755
347.550	0.0	1.11540 04	1.11420 04	12.6304	0.1132	2.6423
373.550	0.0	1.00550 04	1.0057C 04	-1.6494	-0.0164	-0.3451
398.450	0.0	8.92690 03	8.94200 03	-15.1334	-0.1695	-3.1659
417.750	0.0	7.99470 03	7.9830D 03	11.7039	0.1464	2.4484
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.4402	0.0056	0.0921
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				9.5646	0.1037	2.0009

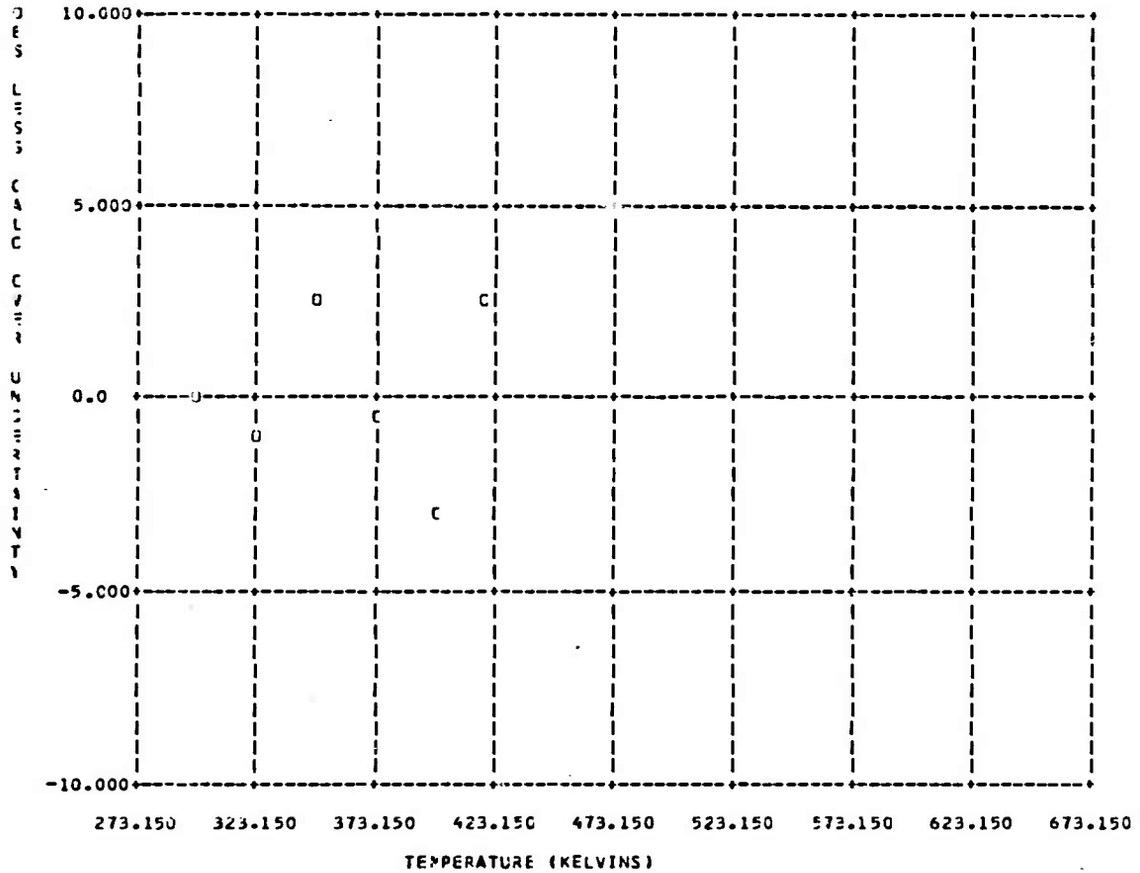
THE NUMBER OF OBSERVATIONS IS 6

10/31/73----------

PHASE	CHLF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2O (L)	-1.000	2.35650070 C1 -1.06954780 C3	-1.7282928D-02	0.0	-5.76916550 04	-1.09719290 02	5.24229760-05
H+	1.000	0.0 0.0	0.0	0.0	0.0	0.0	0.0
OH-	1.000	3.53176540 C2 0.0	-3.5670583D-01	-1.55304120 07	-1.64048200 05	-1.88952970 03	0.0
		'A'/'G'	'B'/'GI1ON1'	'C'	'D'	'E'	'F'
REACTION CONSTANTS		3.29611530 C2 1.06954780 C3	-3.3942690D-01 -1.5530412D 07	0.0	-1.06356540 05	-1.77981040 03	-5.24229760-05

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

H2O = OH- + H+, HEAT OF IONIZATION CLOFSSON AND CLOFSSON, 1973.



PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

TEMPERATURE T(2)	TEMPERATURE T(1)	LOG K OBSERVED	LOG K CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYO
LOG KW			BIGNOLD, PREWER, AND HEARN, 1971.			
324.150	0.0	-1.32410 01	-1.32560 01	0.C150	0.1129	0.7120
334.050	0.0	-1.29920 01	-1.30180 01	0.C259	0.1993	1.2231
343.650	0.0	-1.28C20 01	-1.28080 01	0.C059	0.0462	0.4551
353.350	0.0	-1.26420 01	-1.26140 01	-0.C280	-0.2219	-2.8047
363.050	0.0	-1.24900 01	-1.24370 01	-0.C532	-0.4261	-1.9006
372.450	0.0	-1.22740 01	-1.22800 01	0.C459	0.3754	1.1778
381.750	0.0	-1.20750 01	-1.21390 01	0.C641	0.5312	2.5655
391.150	0.0	-1.19860 01	-1.20080 01	0.C216	0.1803	1.5440
400.450	0.0	-1.18700 01	-1.18900 01	0.C205	0.1724	1.4614
409.850	0.0	-1.17670 01	-1.17820 01	0.C152	0.1296	0.7625
419.150	0.0	-1.17210 01	-1.16860 01	-0.C348	-0.2970	-1.4502
428.550	0.0	-1.16C80 01	-1.15980 01	-0.C092	-0.0792	-0.5410
437.850	0.0	-1.15480 01	-1.15210 01	-0.C266	-0.2304	-1.7737
447.350	0.0	-1.14730 01	-1.14510 01	-0.C215	-0.1872	-2.6846
456.750	0.0	-1.13930 01	-1.13910 01	-0.C018	-0.0160	-0.2273
466.150	0.0	-1.13330 01	-1.13390 01	0.C067	0.0589	0.4768
475.650	0.0	-1.12750 01	-1.12950 01	0.C162	0.1437	2.0258
485.250	0.0	-1.12590 01	-1.12590 01	0.C003	0.0024	0.0343
494.850	0.0	-1.12280 01	-1.12310 01	0.C023	0.0200	0.2814
504.550	0.0	-1.12160 01	-1.12100 01	-0.C057	-0.0504	-0.7066
514.350	0.0	-1.12020 01	-1.11970 01	-0.C053	-0.0473	-0.6618
524.150	0.0	-1.11960 01	-1.11910 01	-0.C041	-0.0367	-0.4561
534.150	0.0	-1.12040 01	-1.11940 01	-0.C099	-0.0887	-1.1036
544.150	0.0	-1.12200 01	-1.12040 01	-0.C158	-0.1404	-0.9265
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.C010	0.0063	-0.1045
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				0.C251	0.2069	1.3987

THE NUMBER OF OBSERVATIONS IS 24

10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2O (L)	-1.000	2.35650070 01 -1.06954780 03	-1.7282928D-02	0.0	-5.76916550 04	-1.09719290 02	5.24229760-05
H+	1.000	0.0 0.0	0.0	0.0	0.0	0.0	0.0
OH-	1.000	3.53176540 02 0.0	-3.5670983D-01	-1.55304120 07	-1.64048200 05	-1.88952970 03	0.0

	'A'/'G'	'B'/'G(ION)'	'C'	'D'	'E'	'F'

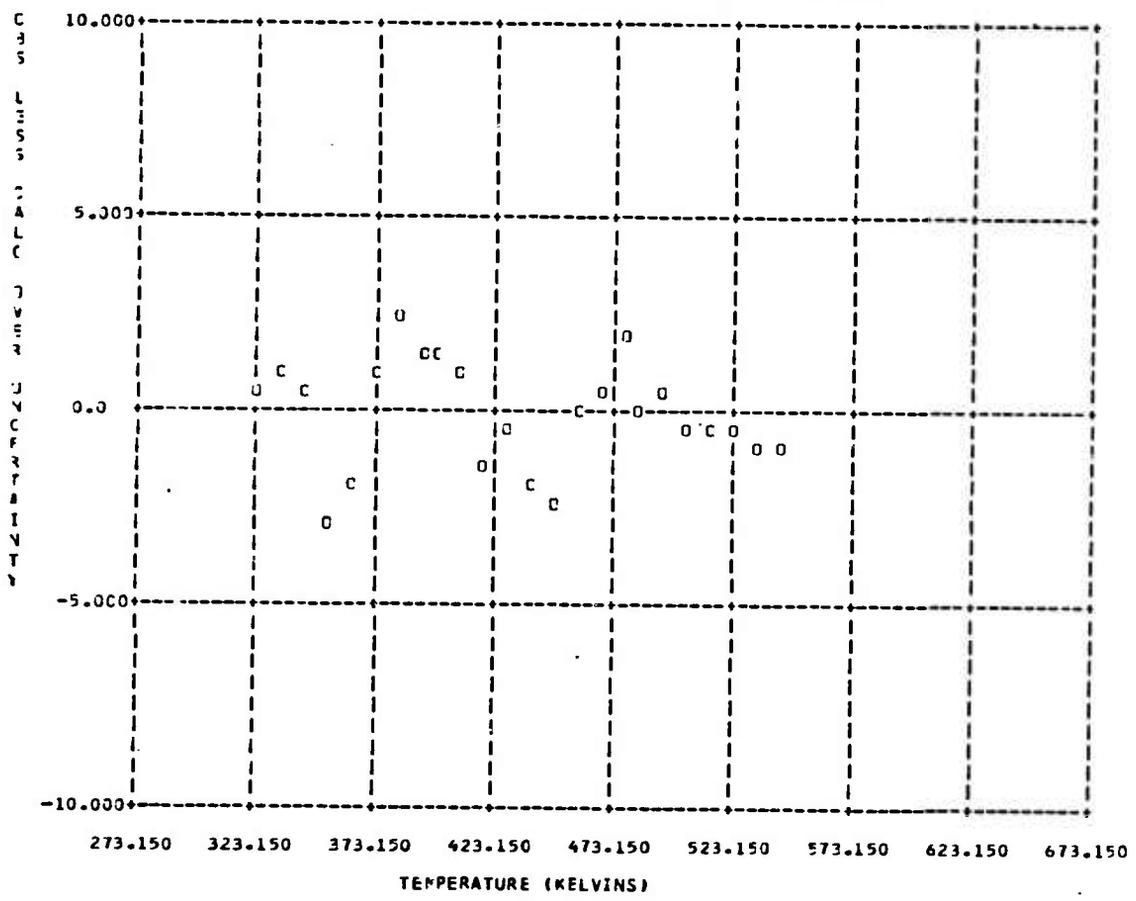
REACTION CONSTANTS	3.29611530 02	-3.39426900-01	0.0	-1.06356540 05	-1.77981040 03	-5.24229760-05
	1.06954780 03	-1.55304120 07				

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

10/31/73

LOG Kw

BIGNOLD, BREWER, AND HEARN, 1971.



PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER. 10/31/73

TEMPERATURE		LOG K		ERROR		
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT	OBS-CALC/SIGYO
H2O = OH- + H+, LOG KW.		SWEETON, MESMER & BAES, PERS COMM, 1973.				
273.150	0.0	-1.49410 01	-1.49510 01	0.0102	0.0680	1.1282
323.150	0.0	-1.32720 01	-1.32810 01	0.0093	0.0701	1.5512
373.150	0.0	-1.22640 01	-1.22690 01	0.0051	0.0418	0.5698
423.150	0.0	-1.16420 01	-1.16480 01	0.0055	0.0475	0.4610
473.150	0.0	-1.13020 01	-1.13060 01	0.0040	0.0355	0.3242
523.150	0.0	-1.11560 01	-1.11920 01	-0.0043	-0.0385	-0.2875
573.150	0.0	-1.13010 01	-1.12750 01	-0.0255	-0.2257	-0.5669
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.0006	-0.0002	0.4557
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				0.0115	0.0980	0.6843

THE NUMBER OF OBSERVATIONS IS 7

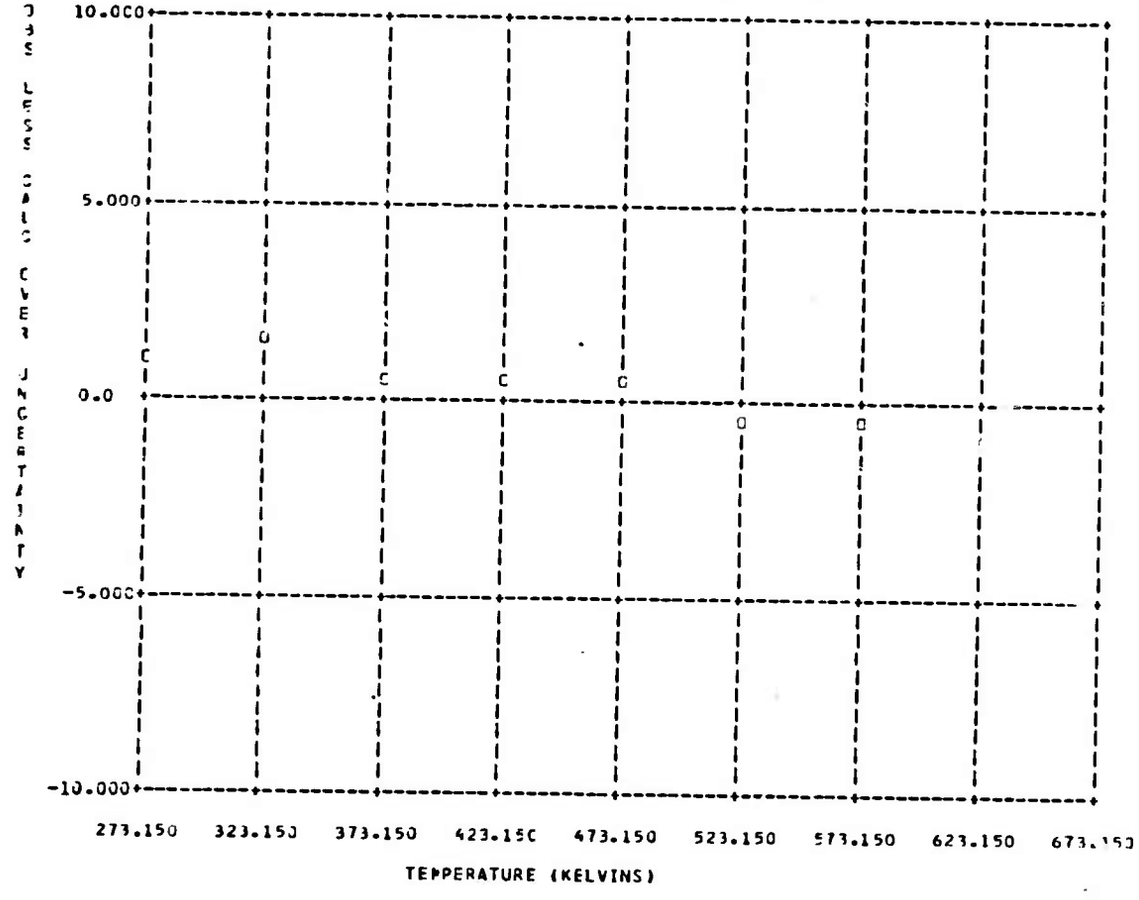
10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2O (L)	-1.000	2.35650370 01 -1.06954780 03	-1.72829280-02	0.0	-5.76916550 04	-1.09719290 02	5.24229780-05
H+	1.000	0.0 0.0	0.0	0.0	0.0	0.0	0.0
OH-	1.000	3.53176540 02 0.0	-3.56709830-01	-1.55304120 07	-1.64048200 05	-1.88952970 03	0.0
		'A'/'G'	'B'/'G(ION)'	'C'	'D'	'E'	'F'
REACTION CONSTANTS		3.29611530 02 1.06954780 03	-3.39426500-01 -1.55304120 07	0.0	-1.06356540 05	-1.77981040 03	-5.24229780-05

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

10/31/73

H2O = OH- + H+, LOG KW. SWEETON, MESMER & BAES, PERS COMM, 1973.



THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

H2O (G)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	7.985	44.404	-41389.	-53517.	42.8158	2.3207	-200.
298.15	8.023	45.105	-41188.	-54636.	40.0496	2.3692	0.
400.00	8.193	47.485	-40362.	-59357.	32.4312	2.5739	825.
500.00	8.409	49.335	-39533.	-64201.	28.0623	2.7840	1655.
600.00	8.667	50.891	-38680.	-69214.	25.2113	3.0014	2509.
700.00	8.952	52.248	-37799.	-74373.	23.2202	3.2251	3389.
800.00	9.250	53.463	-36889.	-79659.	21.7619	3.4543	4299.
900.00	9.554	54.570	-35949.	-85062.	20.6558	3.6886	5240.
1000.00	9.857	55.592	-34978.	-90571.	19.7942	3.9274	6210.
1100.00	10.154	56.546	-33978.	-96178.	19.1088	4.1706	7211.
1200.00	10.442	57.442	-32948.	-101878.	18.5545	4.4178	8241.
1300.00	10.718	58.288	-31890.	-107665.	18.1001	4.6687	9299.
1400.00	10.981	59.092	-30805.	-113534.	17.7234	4.9232	10384.
1500.00	11.229	59.859	-29694.	-119482.	17.4085	5.1811	11495.
1600.00	11.461	60.591	-28559.	-125505.	17.1431	5.4423	12629.
1700.00	11.676	61.292	-27402.	-131599.	16.9182	5.7066	13786.
1800.00	11.873	61.965	-26225.	-137762.	16.7266	5.9738	14964.
1900.00	12.052	62.612	-25028.	-143991.	16.5627	6.2439	16160.
2000.00	12.211	63.234	-23815.	-150284.	16.4222	6.5168	17374.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

H2O (L)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	18.105	15.051	-52185.	-56296.	45.0432	2.4412	C.
298.15	18.006	16.631	-51734.	-56693.	41.5568	2.4584	0.
323.15	17.976	18.080	-51284.	-57127.	38.6354	2.4772	C.
348.15	18.016	19.420	-50835.	-57596.	36.1555	2.4975	C.
373.15	18.128	20.673	-50383.	-58097.	34.0268	2.5193	0.
398.15	18.316	21.854	-49928.	-58629.	32.1821	2.5423	C.
423.15	18.584	22.977	-49466.	-59189.	30.5702	2.5666	0.
448.15	18.944	24.054	-48998.	-59777.	29.1516	2.5921	C.
473.15	19.414	25.094	-48518.	-60392.	27.8951	2.6188	C.
498.15	20.033	26.109	-48026.	-61032.	26.7760	2.6465	C.
523.15	20.875	27.109	-47515.	-61697.	25.7744	2.6754	C.
548.15	22.102	28.110	-46979.	-62387.	24.8740	2.7053	0.
573.15	24.075	29.135	-46404.	-63103.	24.0619	2.7363	0.
598.15	27.682	30.231	-45762.	-63845.	23.3273	2.7685	C.
623.15	35.393	31.500	-44987.	-64616.	22.6618	2.8019	0.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
2.3565007D 01	-1.7282928D-02	0.0	-5.7691655D 04	-1.0971929D 02	5.2422976D-05	-1.0655478D 03

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS FN	LOG K	CELL EMF	PT2-PT1
273.15	0.0	0.0	0.	0.	0.0	0.0	0.
298.15	0.0	0.0	0.	0.	0.0	0.0	0.
323.15	0.0	0.0	0.	0.	0.0	0.0	0.
348.15	0.0	0.0	0.	0.	0.0	0.0	0.
373.15	0.0	0.0	0.	0.	0.0	0.0	0.
398.15	0.0	0.0	0.	0.	0.0	0.0	0.
423.15	0.0	0.0	0.	0.	0.0	0.0	0.
448.15	0.0	0.0	0.	0.	0.0	0.0	0.
473.15	0.0	0.0	0.	0.	0.0	0.0	0.
498.15	0.0	0.0	0.	0.	0.0	0.0	0.
523.15	0.0	0.0	0.	0.	0.0	0.0	0.
548.15	0.0	0.0	0.	0.	0.0	0.0	0.
573.15	0.0	0.0	0.	0.	0.0	0.0	0.
598.15	0.0	0.0	0.	0.	0.0	0.0	0.
623.15	0.0	0.0	0.	0.	0.0	0.0	0.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
0.0	0.0	0.0	0.0	0.0	0.0	0.0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CH-

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS FN	LOG K	CELL EMF	PT2-PT1
273.15	-49.846	1.004	-37336.	-37610.	30.0920	1.6309	0.
298.15	-34.238	-2.624	-38369.	-37586.	27.5514	1.6299	0.
323.15	-26.087	-5.015	-39109.	-37489.	25.3541	1.6256	0.
348.15	-23.330	-6.829	-39718.	-37340.	23.4401	1.6192	0.
373.15	-24.572	-8.470	-40309.	-37149.	21.7576	1.6109	0.
398.15	-28.841	-10.186	-40971.	-36916.	20.2637	1.6008	0.
423.15	-35.442	-12.131	-41771.	-36638.	18.9227	1.5887	0.
448.15	-43.870	-14.397	-42759.	-36307.	17.7057	1.5744	0.
473.15	-53.750	-17.038	-43976.	-35915.	16.5891	1.5574	0.
498.15	-64.797	-20.083	-45456.	-35451.	15.5534	1.5373	0.
523.15	-76.794	-23.544	-47224.	-34907.	14.5827	1.5137	0.
548.15	-89.572	-27.422	-49302.	-34271.	13.6639	1.4861	0.
573.15	-102.997	-31.712	-51708.	-33533.	12.7864	1.4541	0.
598.15	-116.963	-36.403	-54456.	-32682.	11.9412	1.4172	0.
623.15	-131.385	-41.484	-57560.	-31709.	11.1209	1.3750	0.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
3.53176540 02	-3.56709930-01	-1.55304120 07	-1.640482CD 05	-1.88952970 03	0.0	0.0

Problem 2. The System Ni-O and the thermodynamics of Bunsenite (NiO).

As a second example, consider the selected calorimetric data for the following phases for the System Ni-O:

Ni (A)[3]	T<631 K (Curie pernt)
Ni (B)[3]	T>631 K
Bunsenite[3]	T<525 K (Curie pernt)
NiO (B)[3]	525 K<T<565 K (Transition point)
NiO (C)	T>565 K
O_2(G)	ideal gas, all T

The constants for nickel and oxygen are derived from an earlier regression and not refined in this problem. Only refined are the constants for Bunsenite, NiO(B), and NiO(C).

The data are the results of studies by E.G. King and his associates and include:

1. Cp (Bunsenite) from low temperature calorimetry
2. S_{298}(Bunsenite) from third law evaluation of low temperature calorimetry.
3. H(T)-H(298) of Bunsenite from drop calorimetry.
4. H(T) of NiO(B) - H(298) of Bunsenite from drop calorimetry.
5. H(T) of NiO(C)-H(298) of Bunsenite from drop calorimetry.
6. ΔH°_f of Bunsenite from combustion calorimetry.

The input and results for this problem are given below.

Listing of input deck. The next two pages contain a listing of the input deck. Deleted from the input are the constants for Ni(A), Ni(B), and O_2(G) which were in the format (7A8).

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[3] There is no first-order structural change at the Curie pernt. However, because Cp_i is discontinuous, the mathematical model requires separate algebraic expressions for the temperature regions above and below the Curie pernt. The Curie pernt (and also all similar phenomenon) are treated here as "first" order transitions with mathematically derived ΔH and ΔS of "inversion" to describe the local anomaly.

```
10/31/73
    1
PROBLEM 2,  THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.
    1    3    0    0    1
    6    0    0
NI   (A)NI   (B)BUNSENITNIO   (B)NIO   (C)O2   (G)
 1 0 0 0 0 1
    6
BUNSENITE, HEAT CAPACITY                          KING, E. G., JACS 79, 1957.
    1   10    1    1    1    0
BUNSENIT   1.0000 00                        0    0
  206.13D 00              8.13400 00                0.001000 00
  216.19D 00              8.45700 00                0.001000 00
  225.85D 00              8.76200 00                0.001000 00
  236.07D 00              9.05000 00                0.001000 00
  245.63D 00              9.30600 00                0.001000 00
  256.29D 00              9.59700 00                0.001000 00
  266.15D 00              9.84500 00                0.001000 00
  276.01D 00             10.08000 00                0.001000 00
  286.43D 00             10.32000 00                0.001000 00
  295.94D 00             10.55000 00                0.001000 00
BUNSENITE, ENTROPY                                KING, E. G.,  JACS 79, 1957.
    1    1    2    1    1    1
BUNSENITE  1.0000 00                        0    0
  298.15D 00              9.03000 00                0.040000 00
BUNSENITE, RELATIVE HEAT CONTENT.                 KING & CHRISTENSEN, JACS, 1958.
    2    5    7    1    1    0
BUNSENITE -1.0000 00                        0    0
BUNSENITE  1.0000 00                        0    0
  364.90D 00              0.75000 03                0.002000 00
  433.00D 00              1.58000 03                0.002000 00
  502.90D 00              2.58500 03                0.002000 00
  513.20D 00              2.74000 03                0.002000 00
  524.20D 00              2.92500 03                0.002000 00
NICKEL OXIDE, RELATIVE HEAT CONTENT               KING AND CHRISTENSEN, JACS, 1958.
    2    5    7    1    1    0
NIO  (P)   1.0000 00                        0    1
  525.00D 00  565.000 00
        BUNSENITNIO   (B)NIO   (C)
BUNSENITE -1.0000 00                        0    0
  535.50D 00              3.08000 03                0.002000 00
  544.60D 00              3.20500 03                0.002000 00
  554.20D 00              3.33500 03                0.002000 00
  556.20D 00              3.34500 03                0.002000 00
  561.20D 00              3.44500 03                0.002000 00
NICKEL OXIDE, RELATIVE HEAT CONTENT.              KING AND CHRISTENSEN, JACS, 1958.
    2   14    7    1    1    0
NIO  (C)   1.0000 00                        0    2
  525.00D 00  565.00D 00
        BUNSENITNIO   (B)NIO   (C)
BUNSENITE -1.0000 00                        0    0
  572.30D 00              3.58500 03                0.002000 00
  672.30D 00              4.86500 03                0.002000 00
  795.70D 00              6.31500 03                0.002000 00
  873.30D 00              7.44000 03                0.002000 00
  964.90D 00              8.62000 03                0.002000 00
 1088.80D 00             10.21000 03                0.002000 00
 1206.90D 00             11.75000 03                0.002000 00
 1224.40D 00             12.02000 03                0.002000 00
 1304.30D 00             13.12000 03                0.002000 00
```

```
 1406.300 00              14.54000 03              0.002000 00
 1500.900 00              15.84000 03              0.002000 00
 1604.400 00              17.36000 03              0.002000 00
 1706.800 00              18.89000 03              0.002000 00
 1809.700 00              20.44000 03              0.002000 00
BUNSENITE, HEAT OF FORMATION.              BOYLE, KING, AND CONWAY, 1954.
    3    1    3    1    1    1
BUNSENIT   1.0000 00                  0    0
NI    (A)  -1.0000 00                  1    0
02    (G)  -0.5000 00                  1    0
  298.150 00             - 57.3000 03              0.100000 03
110001
(A-FORMATED CONSTANTS FROM RUN ON 10/4/73.  NOT LISTED)          10/ 4/73NI    (A)
(A-FORMATED CONSTANTS FROM RUN ON 10/4/73.  NOT LISTED)          10/ 4/73NI    (B)
 1.000000 01 1.000000-08 1.000000-08 1.000000-08 1.000000 01 1.000000-08BUNSENIT
 1.000000-08                                                              BUNSENIT
 1.000000 01 0.0          0.0          0.0          1.000000 01 0.0          NIO   (B)
 0.0                                                                      NIO   (B)
 1.000000 01 1.000000-08 1.000000-08 0.0          1.000000 01 0.0          NIO   (C)
 0.0                                                                      NIO   (C)
(A-FORMATED CONSTANTS FROM RUN ON 10/4/73.  NOT LISTED)          10/ 4/7302    (G)
0000000000000011111111000100111010000000
    4   10    7   10
 2.0000 03 2.5000 02 1.0000 01
```

Printed output. The following pages contain a complete printed output from the execution of PHAS20 using the **preceding** data deck. By setting IL to 0, the results of the intermediate refinements were deleted. Constant 18, corresponding to the "d" constant for bunsenite, is the least significant of the constants included in the regression. If ICY had been set equal to or greater than 1, this constant would have automatically been set to 0.0 and the regression rerun.

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

PHASES CONSIDERED IN THIS REGRESSION ARE AS FOLLOWS---

NI	(A)	NI	(B)	BUNSENIT	NIO	(B)	NIO (C)
O2	(G)						

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

THE FOLLOWING DATA SETS HAVE BEEN READ IN TO STORAGE:

SET NUMBER REFERENCE

****

1 BUNSENITE, HEAT CAPACITY KING, E. G., JACS 79, 1957.

THE NUMBER OF PHASES IS: 1
THE NUMBER OF OBSERVATIONS IS: 10
THE TYPE OF DATA IS: HEAT CAP

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BUNSENIT	1.000	NO	0

INDEX	TEMPERATURE T2	T1	HEAT CAP	ERROR
1	206.130	-	8.134000 00	8.134000-03
2	216.190	-	8.457000 00	8.457000-03
3	225.850	-	8.762000 00	8.762000-03
4	236.070	-	9.050000 00	9.050000-03
5	245.630	-	9.306000 00	9.306000-03
6	256.290	-	9.597000 00	9.597000-03
7	266.150	-	9.845000 00	9.845000-03
8	276.010	-	1.008000 01	1.008000-02
9	286.430	-	1.032000 01	1.032000-02
10	295.940	-	1.055000 01	1.055000-02

****

2 BUNSENITE, ENTROPY KING, E. G., JACS 79, 1957.

THE NUMBER OF PHASES IS: 1
THE NUMBER OF OBSERVATIONS IS: 1
THE TYPE OF DATA IS: ENTROPY

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BUNSENIT	1.000	NO	0

INDEX	TEMPERATURE T2	T1	ENTROPY	ERROR
11	298.150	-	9.080000 00	4.000000-02

****

3 BUNSENITE, RELATIVE HEAT CONTENT. KING & CHRISTENSEN, JACS, 1958.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 5
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BUNSENIT	-1.000	NO	0
BLASENIT	1.000	NO	0

INDEX	TEMPERATURE T2	TEMPERATURE T1	HT2-HT1	ERROR
12	364.900	298.150	7.500000 02	1.500000 00
13	432.000	298.150	1.580000 03	3.160000 00
14	502.900	298.150	2.585000 03	5.170000 00
15	513.200	298.150	2.740000 03	5.480000 00
16	524.200	298.150	2.925000 03	5.850000 00

****

4 NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 5
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
NIO (B)	1.000	NO	1

INVERSIONS ARE AS FOLLOWS:

1.00 BUNSENIT = NIO (B) 525.000

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BLASENIT	-1.000	NO	0

INDEX	TEMPERATURE T2	TEMPERATURE T1	HT2-HT1	ERROR
17	535.500	298.150	3.080000 03	6.160000 00
18	544.600	298.150	3.205000 03	6.410000 00
19	554.200	298.150	3.335000 03	6.670000 00
20	556.200	298.150	3.345000 03	6.690000 00
21	561.200	298.150	3.445000 03	6.890000 00

****

5 NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 14
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
NIO (C)	1.000	NO	2

INVERSIONS ARE AS FOLLOWS:

1.00 BUNSENIT = NIO (B) 525.000
1.00 NIO (B) = NIO (C) 565.000
BUNSENIT -1.000 AC 0

INDEX	TEMPERATURE T2	T1	HT2-HT1	ERROR
22	572.300	298.150	3.585CCO 03	7.170CCO 00
23	672.300	298.150	4.865C00 03	9.730CCO CO
24	785.700	298.150	6.315C00 03	1.263C00 01
25	873.300	298.150	7.44CCOO 03	1.488C0D 01
26	964.900	298.150	8.62CCOC 03	1.724CC0 01
27	1088.800	298.150	1.021C0C 04	2.042C0D C1
28	1204.900	298.150	1.175CCC 04	2.35CCJO 01
29	1224.400	298.150	1.202000 04	2.404C30 01
30	1304.300	298.150	1.312CCD 04	2.624C0D C1
31	1406.300	298.150	1.454C00 04	2.9C8000 01
32	1506.900	298.150	1.584CCC 04	3.168C00 01
33	1604.400	298.150	1.736C0D 04	3.472C0D 01
34	1706.800	298.150	1.889000 04	3.778000 01
35	1805.700	298.150	2.044000 04	4.088CC0 01

****

6 BUNSENITE, HEAT OF FORMATION. BOYLE, KING, AND CONWAY, 1954.

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 1
THE TYPE OF DATA IS: ENTHALPY

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BUNSENIT	1.000	AC	C
NI (A)	-1.000	YES	C
C2 (G)	-0.500	YES	C

INDEX	TEMPERATURE T2	T1	ENTHALPY	ERROR
36	298.150	-	-5.730000 04	1.000000 02

THE INDEX OF THE LAST ITEM OF THE ABOVE DATA SETS IN THE VECTORS X(1,I), YC(I), AND SIGYO(I) IS AS FOLLOWS:

DATA SET	INDEX
1	10
2	11
3	16
4	21
5	35
6	36

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

NUMBER OF CYCLES IN THIS JOB IS 3

NUMBER OF PARAMETERS TO BE VARIED IS 13

NUMBER OF INDEPENDENT VARIABLES PER OBSERVATION IS 2

DERIVATIVES PROGRAMMED IN SUBROUTINE EAFW20.

WEIGHTS TO BE SUPPLIED BY USER

NUMBER OF PARAMETERS READ IS 42

NUMBER OF OBSERVATIONS READ IS 36

TOTAL CONSTANTS

I	P(I)	KI(I)
	NI (A)	
1	1.37040 01	0
2	-1.29020-02	0
3	-2.16220 05	0
4	0.0	0
5	-6.57710 01	0
6	2.97700-05	0
7	0.0	0
	NI (B)	
8	-3.10550 00	0
9	6.81490-03	0
10	1.47600 06	0
11	0.0	0
12	2.66100 01	0
13	-4.13150-06	0
14	0.0	0
	BUNSENIT	
15	1.00000 01	1
16	1.00000-08	1
17	1.00000-08	1
18	1.00000-08	1
19	1.00000 01	1
20	1.00000-08	1
21	1.00000-08	1
	NIO (B)	
22	1.00000 01	1
23	0.0	0
24	0.0	0
25	0.0	0
26	1.00000 01	1
27	0.0	0
28	0.0	0
	NIO (C)	
29	1.00000 01	1
30	1.00000-08	1
31	1.00000-08	1

32	0.0	0
33	1.000000 01	1
34	0.0	0
35	0.0	0
	C2 (G)	
36	1.340000 01	0
37	-5.974000-04	0
38	1.619000 05	0
39	0.0	0
40	-4.187800 01	0
41	2.508700-07	0
42	-1.359200 02	0

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

BUNSENITE, HEAT CAPACITY	KING, E. G., JACS 79, 1957.
BUNSENITE, ENTROPY	KING, E. G., JACS 79, 1957.
BUNSENITE, RELATIVE HEAT CONTENT.	KING & CHRISTENSEN, JACS, 1958.
NICKEL OXIDE, RELATIVE HEAT CONTENT	KING AND CHRISTENSEN, JACS, 1958.
NICKEL OXIDE, RELATIVE HEAT CONTENT.	KING AND CHRISTENSEN, JACS, 1958.
BUNSENITE, HEAT OF FORMATION.	BOYLE, KING, AND CONWAY, 1954.

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 0.2790 07

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.3481D 02

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
NI (A)						
1	1.37036280150 01	1.37036280150 C1				
2	-1.29019559040-02	-1.29015559040-C2				
3	-2.16220388110 05	-2.1622C388110 C5				
4	0.0	0.0				
5	-6.57710667810 01	-6.57710667810 C1				
6	2.97700356390-05	2.977C0356390-C5				
7	C.C	0.0				
NI (B)						
8	-3.10546694470 00	-3.10546694470 C0				
9	6.81486261710-03	6.81486261710-C3				
10	1.47599994049D 06	1.4759999C49C C6				
11	0.0	0.0				
12	2.66102409970 01	2.66102409970 C1				
13	-4.13146688060-06	-4.13146688060-C6				
14	0.C	0.0				
BUNSENIT						
15	1.CC00000000000 01	2.17306855320 02	2.27006855320 02	3.96676685180 01	9.5594846651C 01	17.4742
16	1.CC00000000000-08	-1.62995606010-C1	-1.62995960 1C-01	3.0C455540751C-02	1.CC00CC06140 02	18.4139
17	1.CC00000000000-08	8.55305775430 C5	8.5530577543C 05	1.77553136140 C5	1.C0000000C0D C2	20.7490
18	1.CC00000000000-08	-9.81501095410 C3	-9.8150109541C 03	7.58361012710 C3	1.0000000C0D 02	77.2654
19	1.CC00000000000 01	-1.50803827640 03	-1.49803827640 03	2.64566833030 02	1.00667539690 02	17.6609
20	1.CC00000000000-08	2.60904164890-C4	2.60914164890-04	4.4830148032C-C5	9.9996167322C C1	17.1819
21	1.CC00000000000-08	-2.62571055690 C3	-2.6257105569C 03	4.78906814440 02	1.C0000000000 02	18.2291
NIC (B)						
22	1.C0000000000 01	3.72494487270 00	1.3724944873C 01	5.0232688572C-C1	2.7139962362C 01	3.6000
23	0.C	0.0				
24	C.C	0.0				
25	0.C	0.0				
26	1.C0000000000 01	-7.97078635510 C1	-6.9707863551C 01	3.17C48561380 00	1.14345583830 02	4.5482
27	C.C	0.0				
28	C.C	0.0				
NIC (C)						
29	1.C0000000000 01	-1.53143566860 C0	8.4685641314C 00	6.8581137717C-01	-1.8083772465C 01	8.1456
30	1.C0000000000-08	1.82396744CC0-03	1.82397744CCC-03	2.2196508223C-04	9.9999451748C 01	12.1693
31	1.C0000000000-08	8.36545797290 05	8.3654579729D 05	2.0180248277C 05	1.0000000C0C 02	24.1232
32	C.C	0.0				
33	1.C0000000000 01	-4.71432741140 C1	-3.71432741140 01	4.4242527545D C0	1.2692277468D 02	11.9113
34	C.C	0.0				
35	0.C	0.0				
O2 (C)						
36	1.34086510000 01	1.3408E510000 C1				
37	-5.97401480000-04	-5.974C14[illegible]000-C4				
38	1.61901710000 05	1.6190171[illegible]00 C5				
39	C.C	0.0				
40	-4.18778890000 01	-4.1877E8900C0 C1				
41	2.50889120000-07	2.5088S120CC0-C7				
42	-1.35920060000 02	-1.3592CC60C00 C2				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

SUM(W*(O-C)**2) IS 0.5880 C2

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.1559 C1

PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

BUNSENITE, HEAT CAPACITY	KING, E. G., JACS 79, 1957.
BUNSENITE, ENTROPY	KING, E. G., JACS 79, 1957.
BUNSENITE, RELATIVE HEAT CONTENT.	KING & CHRISTENSEN, JACS, 1958.
NICKEL OXIDE, RELATIVE HEAT CONTENT	KING AND CHRISTENSEN, JACS, 1958.
NICKEL OXIDE, RELATIVE HEAT CONTENT.	KING AND CHRISTENSEN, JACS, 1958.
BUNSENITE, HEAT OF FORMATION.	BOYLE, KING, AND CONWAY, 1954.

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 2

SUM(W*(O-C)**2) IS 0.5940 02

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.1607D 01

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

PARAMETERS AFTER LEAST SQUARES CYCLE 2

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
NI (A)						
1	1.37036280150 01	1.37036280150 C1				
2	-1.29019559040-02	-1.29019559040-C2				
3	-2.16220388110 05	-2.1622C38811D C5				
4	C.C	0.0				
5	-6.5771C66781D 01	-6.5771C66781C C1				
6	2.9770335639D-05	2.9770335639D-C5				
7	C.C	0.0				
NI (B)						
8	-3.10546549470 00	-3.10546549470 C0				
9	6.81486261710-03	6.81486261710-C3				
10	1.4759[illegible]0490 06	1.4759559C490 C6				
11	C.C	0.0				
12	2.66102409970 01	2.66102409970 C1				
13	-4.13146688060-06	-4.13146688060-C6				
14	C.C	0.0				
BUNSENIT						
15	2.27006855320 02	1.73891.82660-06	2.27006857C6C 02	3.58765042760 C1	7.66017312530-07	17.5[illegible]2
16	-1.62596596310-01	-1.05805485970-C9	-1.62960597C7C-01	3.02037195280-02	6.49175399530-C7	18.5309
17	8.55300775430 05	8.78206404320-C3	8.5530576421C 05	1.7848789843C C5	1.0267747752C-06	20.8683
18	-9.81501099410 03	2.49206625060-C4	-9.8150107049C 03	7.62353505930 C3	-2.5390356930D-C6	77.6722
19	-1.49803827640 03	-6.5528E373G70-C6	-1.4980382829C 03	2.6595968C59C 02	4.3743095261C-07	17.7539
20	2.6091[illegible]164890-04	1.48683260750-12	2.6091416637C-04	4.5C66162356C-05	5.6985507056C-07	17.2724
21	-2.62571055690 03	-1.50494116140-05	-2.6257105720C 03	4.8142808357C 02	5.7315576875C-C7	18.[illegible]351
NIO (B)						
22	1.37249448730 01	1.38835338790-C8	1.3724944887C 01	5.C497145295C-01	1.0115839439C-C7	3.6792
23	C.C	0.0				
24	0.C	0.0				
25	0.0	0.0				
26	-6.9707863551C 01	-8.75773785170-08	-6.9707863638C 01	3.18717706C3C 00	1.2563486233D-07	4.5722
27	C.0	0.0				
28	C.C	0.0				
NIO (C)						
29	8.46856413140 00	-2.1810E074380-C8	8.4685641056C 00	6.9344298163C-01	-2.5755024294C-07	8.1884
30	1.8239774440D-03	6.566C5826750-12	1.8239774469C-03	2.2313364716C-C4	3.8191581147C-07	12.2334
31	8.3654[illegible]79729D 05	6.26653485320-C3	8.365458C355C 05	2.0286489899C 05	7.4909286054C-07	24.2502
32	0.C	0.0				
33	-3.71432741140 01	1.3983C653380-C7	-3.7143273974C 01	4.44754486650 00	-3.76462918890-07	11.9740
34	C.C	0.0				
35	C.C	0.0				
O2 (G)						
36	1.34J86510000 01	1.3408651C0CC C1				
37	-5.5740148J000-04	-5.9740148DJC0-C4				
38	1.6193171000D 05	1.61901710CCC C5				
39	C.C	0.0				
40	-4.18778890000 01	-4.1877889[illegible]C0 C1				
41	2.5088912000D-07	2.5088912000D-C7				
42	-1.3592000600D0 02	-1.3592CC6000D C2				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 2

SUM(W*(C-C)**2) IS 0.5940 02

SQRTF(SUM(W*(J-C)**2)/(NC-NV)) IS 0.1607D 01

PROBLEM 2, THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

BUNSENITE, HEAT CAPACITY	KING, E. G., JACS 79, 1957.
BUNSENITE, ENTROPY	KING, E. G., JACS 79, 1957.
BUNSENITE, RELATIVE HEAT CONTENT.	KING & CHRISTENSEN, JACS, 1958.
NICKEL OXIDE, RELATIVE HEAT CONTENT	KING AND CHRISTENSEN, JACS, 1958.
NICKEL OXIDE, RELATIVE HEAT CONTENT.	KING AND CHRISTENSEN, JACS, 1958.
BUNSENITE, HEAT OF FORMATION.	BOYLE, KING, AND CONWAY, 1954.

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 3

SUM(W*(O-C)**2) IS 0.594D 02

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.1607D 01

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

PARAMETERS AFTER LEAST SQUARES CYCLE 3

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
NI (S)						
1	1.3763628D150 01	1.3703628C15D C1				
2	-1.2901955904D-02	-1.2901955904D-C2				
3	-2.1622C388110 05	-2.1622C38811D C5				
4	C.C	0.0				
5	-6.5771C667810 01	-6.5771C66781D C1				
6	2.9770335650D-05	2.97703356390-C5				
7	0.C	0.0				
NI (B)						
8	-3.1054C54947D 00	-3.1054E54947D CC				
9	6.8148C261710-03	6.8148E261710-C3				
10	1.4759954C490 06	1.4759954C49C C6				
11	C.C	0.0				
12	2.6610240997D 01	2.661024C997D C1				
13	-4.1314C688J6D-06	-4.1314E688C6D-C6				
14	C.C	0.0				
BUNSENIT						
15	2.2700685706D 02	2.95123734500-11	2.2700685706C 02	3.9876504276D C1	1.3000652658D-11	17.5[illegible]62
16	-1.6299059707D-01	-2.2554EC0433D-14	-1.6299059707C-01	3.0203719528C-02	1.3838197319C-11	18.5[illegible]69
17	8.5530578421D 05	1.3368203415D-C7	8.5530578421C 05	1.7648788843C 05	1.5278584027C-11	20.8[illegible]83
18	-9.8150107049D 03	5.82617459240-C9	-9.8150107049C 03	7.6235350593D C3	-5.9359839409C-11	77.6722
19	-1.4980382829D 03	-2.3786E03388D-10	-1.4980382829C 03	2.6595968C59C 02	1.3875882629C-11	17.7[illegible]39
20	2.6091416637D-04	3.34015718920-17	2.6091416637C-04	4.5066162356C-05	1.2801900470D-11	17.2724
21	-2.6257105720D 03	-3.7022E03703D-10	-2.6257105720C 03	4.8142808357D 02	1.4100032234D-11	18.3651
NIC (B)						
22	1.3724944887D 01	-1.7112470618D-14	1.3724944887C 01	5.C497145295D-C1	-1.2468152521C-13	3.6732
23	0.C	0.0				
24	C.C	0.0				
25	C.C	0.0				
26	-6.9707863638D 01	3.3126216872D-14	-6.9707863638C 01	3.1871770603C 00	-4.7521492043D-14	4.5722
27	C.C	0.0				
28	C.C	0.0				
NIC (C)						
29	8.4685641096D 00	-2.8901566338D-14	8.4685641C96C 0C	6.9244298163C-01	-3.4128532257C-13	8.1884
30	1.8239774469D-03	8.4308310135D-18	1.8239774469C-03	2.2313364716D-C4	4.6222232778C-13	12.2434
31	8.3654980355D 05	9.8528C19544D-C9	8.365498C355D 05	2.C2864898990 05	1.1777902466C-12	24.2502
32	C.C	0.0				
33	-3.7143273974D 01	1.1533C629030-13	-3.7143273974C 01	4.4475448665C 00	-3.1050205513C-13	11.9740
34	0.0	0.0				
35	C.C	0.0				
N2 (G)						
36	1.3430865100JD 01	1.3430865100C0 C1				
37	-5.9743148000D-04	-5.9740148000D-C4				
38	1.6190171000D 05	1.6190171000C0 C5				
39	C.C	0.0				
40	-4.1877489000D 01	-4.1877E8900CD C1				
41	2.5088912000D-07	2.5088912000D-C7				
42	-1.3592C060000 02	-1.3592CC60000 C2				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 3

SUM(W*(O-C)**2) IS 0.594D 02

SQRT(SUM(W*(O-C)**2)/(NO-NV)) IS 0.160?D 01

SUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FOR REASON 1

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

CORRELATION MATRIX

1	0.10000 01	-0.99870 00	0.9949D 00	0.9985D 00	-0.10000 01	0.9949D 00	-0.9997D 00	-0.5059D-08	-0.5306D-03	0.5666D-08
	-0.5627D-08	-0.5565D-08	-0.3802D-03							
2	0.0	0.1000D 01	-0.9986D 00	-0.9946D 00	0.9983D 00	-0.9988D 00	0.9971D 00	0.5055D-08	0.5424D-03	-0.5660D-08
	0.5620D-08	0.5557D-08	0.3887D-03							
3	0.0	0.0	0.1000D 01	0.9985D 00	-0.9957D 00	0.9980D 00	-0.9972D 00	-0.5027D-08	-0.5003D-03	0.5639D-08
	-0.5599D-08	-0.5536D-08	-0.3585D-03							
4	0.0	0.0	0.0	0.1000D 01	-0.9988D 00	0.9984D 00	-0.9995D 00	-0.5048D-08	-0.5160D-03	0.5659D-08
	-0.5619D-08	-0.5556D-08	-0.3698D-03							
5	0.0	0.0	0.0	0.0	0.10000 01	-0.9941D 00	0.9958D 00	0.5058D-08	0.5334D-03	-0.5668D-08
	0.5627D-08	0.5564D-08	0.3823D-03							
6	0.0	0.0	0.0	0.0	0.0	0.10000 01	-0.9920D 00	-0.5039D-08	-0.5496D-03	0.5639D-08
	-0.5599D-08	-0.5537D-08	-0.3938D-03							
7	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01	0.5056D-08	0.5236D-03	-0.5666D-08
	0.5625D-08	0.5563D-08	0.3752D-03							
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01	-0.9998D 00	0.5366D-10
	-0.5625D-10	-0.5273D-10	-0.7818D-04							
9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01	-0.5665D-10
	0.5622D-10	0.5567D-10	0.3706D-03							
10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1000D 01
	-0.9941D 00	-0.9979D 00	-0.9997D 00							
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.1000D 01	0.9546D 00	0.9920D 00							
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.1000D 01	0.9830D 00							
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.1000D 01							

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

TEMPERATURE		HEAT CAP		ERROR		
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT	OBS-CALC/SIGYO
BUNSENITE, HEAT CAPACITY		KING, E. G., JACS 79, 1957.				
206.130	0.0	8.134CD 00	8.1440D 00	-0.0100	-0.1234	-1.2341
216.190	0.0	8.457CD 00	8.4491D 00	0.0079	0.0930	0.9305
225.850	0.0	8.762CD 00	8.7431D 00	0.0189	0.2156	2.1559
236.070	0.0	9.05CCD 00	9.0467D 00	0.0033	0.0365	0.3654
245.630	0.0	9.306CD 00	9.3190D 00	-0.0130	-0.1402	-1.4018
256.250	0.0	9.597CD 00	9.6065D 00	-0.0095	-0.0994	-0.9945
266.150	0.0	9.845CD 00	9.8562D 00	-0.0112	-0.1142	-1.1419
276.010	0.0	1.00F0D 01	1.0090D 01	-0.0105	-0.1041	-1.0410
286.430	0.0	1.0320D 01	1.0322D 01	-0.0023	-0.0222	-0.2216
295.940	0.0	1.0550D 01	1.0521D 01	0.0289	0.2738	2.7380
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.0002	0.0015	0.0155
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				0.0137	0.1416	1.4161

THE NUMBER OF OBSERVATIONS IS 10

100

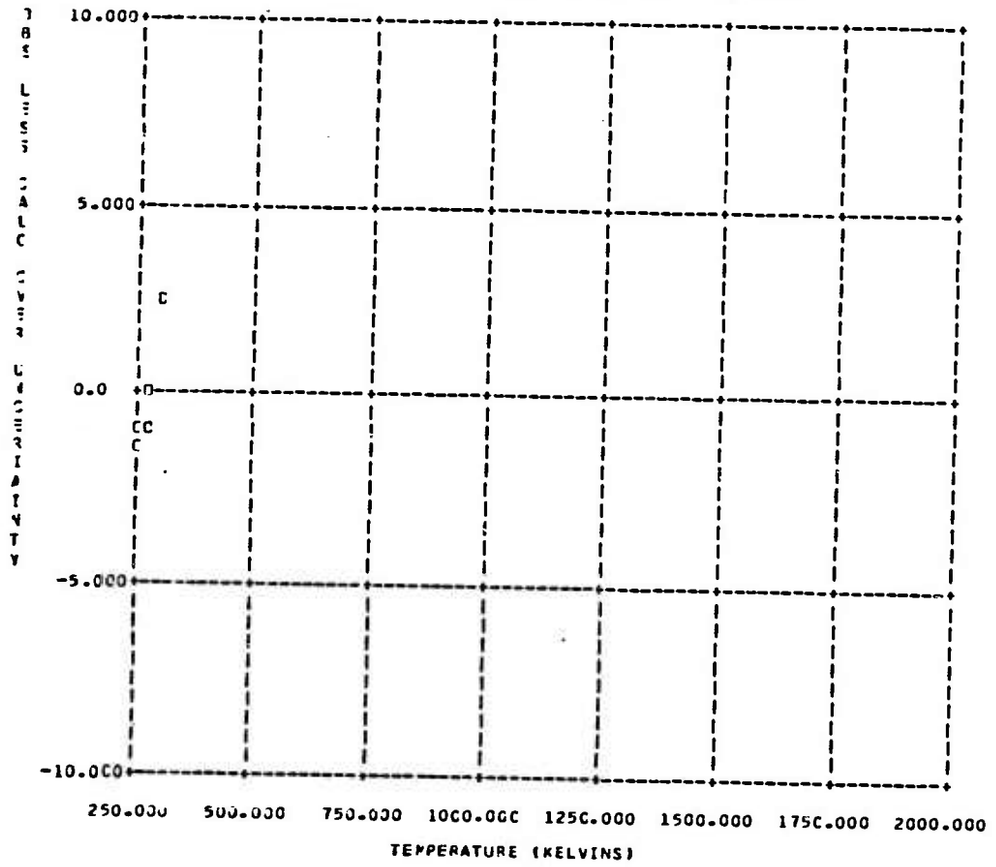
10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
BUNSENIT	1.000	2.27006860 02	-1.62990600-01	8.55305780 05	-9.81501070 03	-1.49803830 03	2.60914170-04
		-2.62571060 03					

PROF EM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

10/31/73

BUNSENITE, HEAT CAPACITY KING, E. G., JACS 79, 1957.



PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

TEMPERATURE		ENTROPY		ERROR		
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT	OBS-CALC/SIGYO
BUNSENITE, ENTROPY		KING, E. G., JACS 79, 1957.				
298.150	0.0	9.08000 00	9.08000 00	0.0000	0.0000	0.0000
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.0000	0.0000	0.0000
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				0.0	0.0	0.0
THE NUMBER OF OBSERVATIONS IS 1						

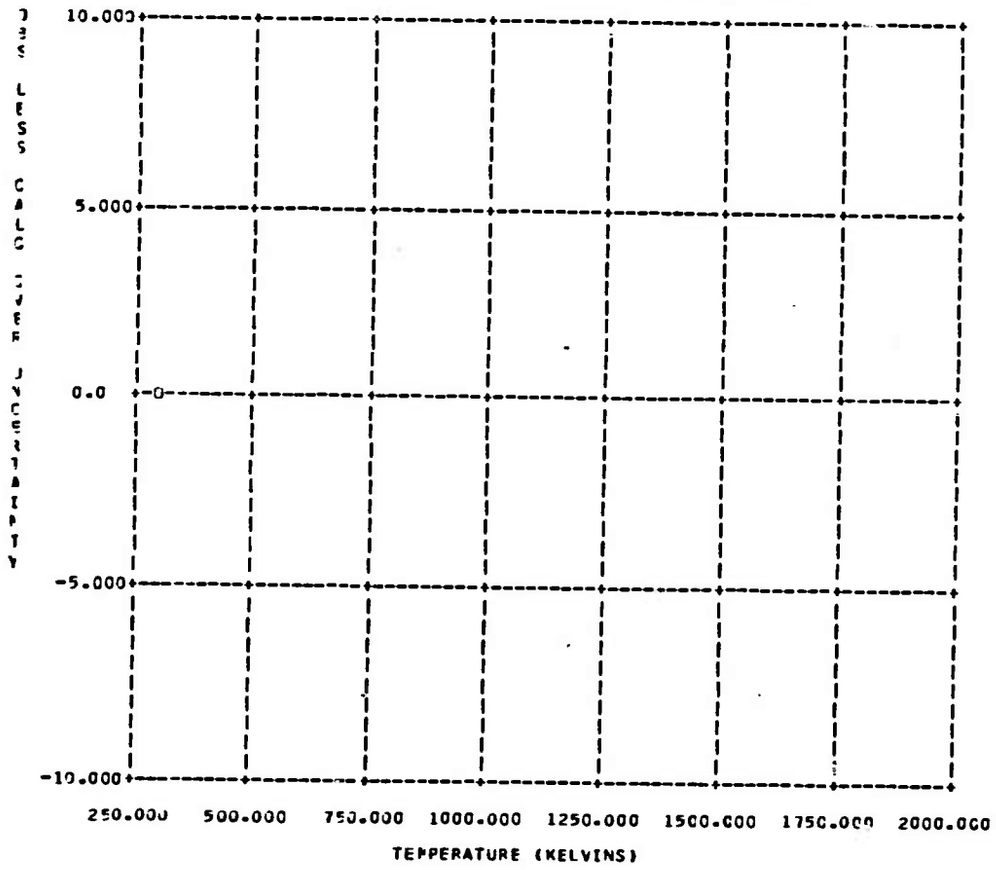
10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
BUNSENIT	1.000	2.27006860 02	-1.62990600-01	8.55305780 05	-9.81501070 03	-1.49803830 03	2.60914170-04
		-2.62571060 03					

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

10/31/73

BUNSENITE, ENTROPY KING, E. G., JACS 79, 1957.



PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

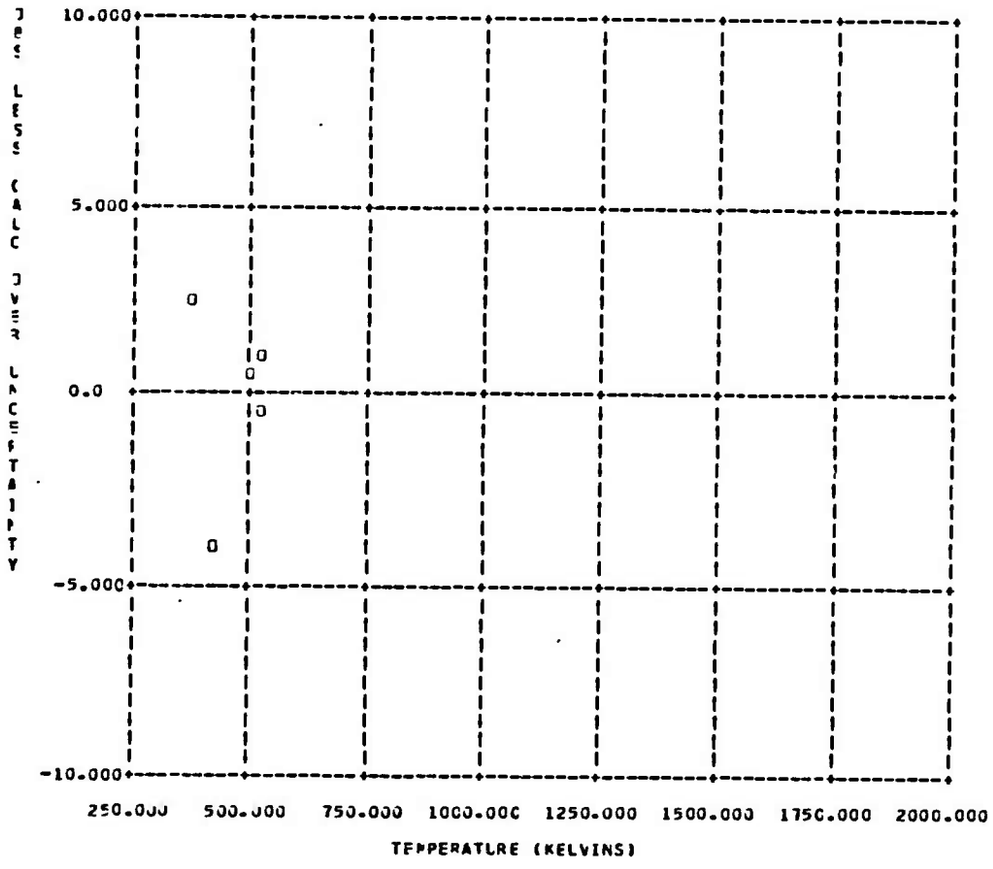
TEMPERATURE T(2)	TEMPERATURE T(1)	HT2-HT1 OBSERVED	HT2-HT1 CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYO
BUNSENITE, RELATIVE HEAT CONTENT.		KING & CHRISTENSEN, JACS, 1958.				
364.900	298.150	7.5000D 02	7.4626D 02	3.7356	0.4986	2.4931
433.000	298.150	1.5800D 03	1.5921D 03	-12.0547	-0.7630	-3.8148
502.900	298.150	2.5850D 03	2.5824D 03	2.6420	0.1022	0.5110
513.200	298.150	2.7400D 03	2.7426D 03	-2.6404	-0.0964	-0.4818
524.200	298.150	2.9250D 03	2.9188D 03	6.2451	0.2135	1.0675
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				-0.4137	-0.0050	-0.0450
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				6.5023	0.4232	2.1162
THE NUMBER OF OBSERVATIONS IS 5						

10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
BUNSENIT	-1.000	2.2700686D 02 -2.6257106D 03	-1.6299060D-01	8.5530578D 05	-9.8150107D 03	-1.4980383D 03	2.6091417D-04
BUNSENIT	1.000	2.2700686D 02 -2.6257106D 03	-1.6299060D-01	8.5530578D 05	-9.8150107D 03	-1.4980383D 03	2.6091417D-04

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

BUNSENITE, RELATIVE HEAT CONTENT. KING & CHRISTENSEN, JACS, 1958.



PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

TEMPERATURE T(2)	TEMPERATURE T(1)	HT2-HT1 OBSERVED	HT2-HT1 CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYO
NICKEL OXIDE, RELATIVE HEAT CONTENT — KING AND CHRISTENSEN, JACS, 1958.						
535.500	298.150	3.08000 03	3.07830 03	1.7429	0.0566	0.2829
544.600	298.150	3.20500 03	3.20320 03	1.8459	0.0576	0.2880
554.200	298.150	3.33500 03	3.33490 03	0.0864	0.0026	0.0130
556.200	298.150	3.34500 03	3.36240 03	-17.3635	-0.5191	-2.5954
561.200	298.150	3.44500 03	3.43100 03	14.0118	0.4067	2.0336
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.0647	0.0039	0.0044
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				10.0424	0.2971	1.4856
THE NUMBER OF OBSERVATIONS IS 5						

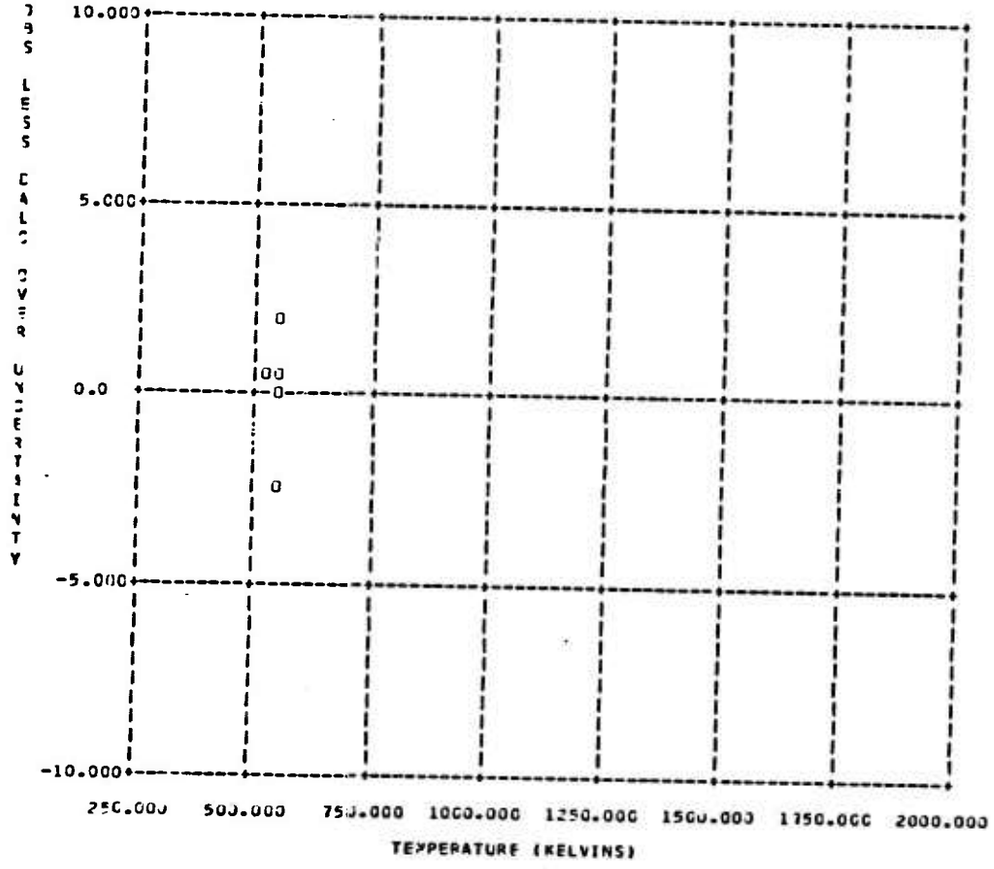
10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
NIC (B)	1.000	1.37249450 01 0.0	0.0	0.0	-5.21332130 04	-6.97078640 01	0.0
BUNSENIT	-1.000	2.27006860 02 -2.62571060 03	-1.62990600-01	8.55305780 05	-9.81501070 03	-1.49803830 03	2.6091417D-04

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

10/31/73

NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.



PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE. 10/31/73

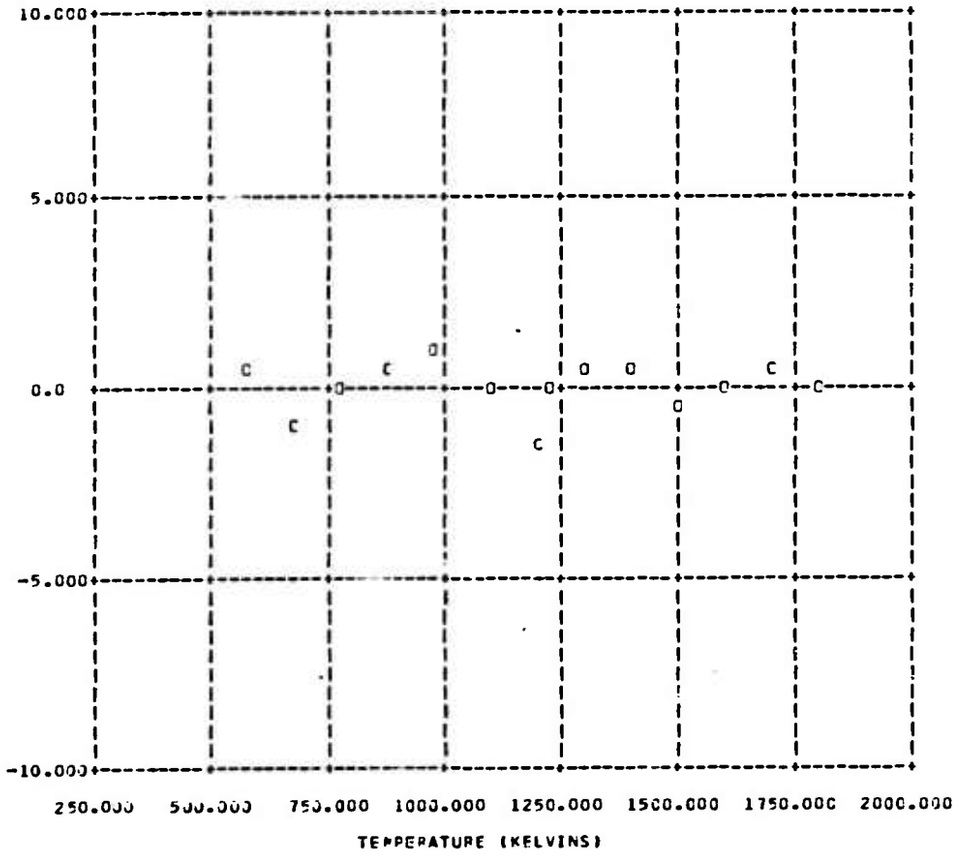
TEMPERATURE T(2)	TEMPERATURE T(1)	HT2-HT1 OBSERVED	HT2-HT1 CALCULATED	ERROR DIFFERENCE	ERROR PERCENT	ERROR OBS-CALC/SIGYO
NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.						
572.300	298.150	3.58500 03	3.58270 03	2.2597	0.0630	0.3152
672.300	298.150	4.86500 03	4.87400 03	-9.0317	-0.1856	-0.9282
785.700	298.150	6.31500 03	6.31550 03	-0.5294	-0.0084	-0.0419
873.300	298.150	7.44000 03	7.42930 03	10.7476	0.1445	0.7223
964.900	298.150	8.62000 03	8.60300 03	16.9702	0.1969	0.9844
1058.800	298.150	1.02100 04	1.02150 04	-5.0603	-0.0496	-0.2478
1206.900	298.150	1.17500 04	1.17850 04	-34.9019	-0.2970	-1.4852
1224.400	298.150	1.20200 04	1.20210 04	-0.6147	-0.0051	-0.0256
1304.300	298.150	1.31200 04	1.31080 04	12.3708	0.0943	0.4714
1406.300	298.150	1.45400 04	1.45220 04	17.7621	0.1222	0.6108
1500.900	298.150	1.58400 04	1.58620 04	-22.4896	-0.1420	-0.7099
1604.400	298.150	1.73600 04	1.73610 04	-1.1654	-0.0067	-0.0336
1706.800	298.150	1.88500 04	1.88780 04	11.9211	0.0631	0.3155
1809.700	298.150	2.04400 04	2.04370 04	2.6348	0.0129	0.0645
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				0.0624	0.0002	0.0008
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				14.2910	0.1301	0.6506
THE NUMBER OF OBSERVATIONS IS 14						

10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
NIO (C)	1.000	8.46856410 C0 0.0	1.82397740-03	8.36549E00 05	-4.82612510 04	-3.71432740 01	0.0
BUNSENIT	-1.000	2.27006860 C2 -2.62571060 C3	-1.62990600-01	8.55305780 05	-9.81501C70 03	-1.49803830 03	2.60914170-04

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE. 10/21/73

NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.



PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF EUNSENITE. 10/31/73

TEMPERATURE		ENTHALPY		ERROR		
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT	OBS-CALC/SIGYO
EUNSENITE, HEAT OF FORMATION.		BOYLE, KING, AND CONWAY, 1954.				
298.150	0.0	-5.73000 04	-5.73000 04	-0.0000	-0.0000	-0.0000
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----				-0.0000	-0.0000	-0.0000
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE ----------				0.0	0.0	0.0

THE NUMBER OF OBSERVATIONS IS 1

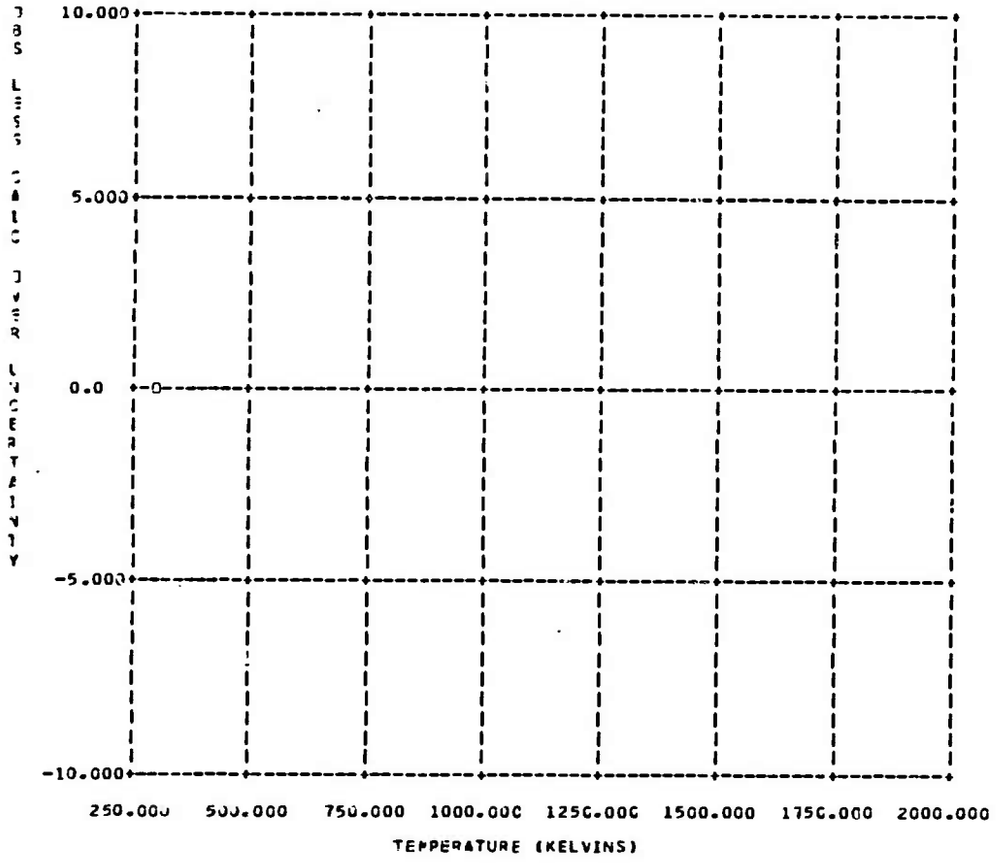
10/31/73----------

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
EUNSENIT	1.000	2.27000686D 02 -2.62571360 02	-1.62990600-01	8.5530578D 05	-9.81501070 03	-1.49803830 03	2.60914170-04
NI (A)	-1.000	1.37033280 01 0.0	-1.29019560-02	-2.1622039D 05	-1.79449520 03	-6.57710670 01	2.977033C0-05
02 (G)	-0.500	1.34086510 01 -1.35920060 02	-5.5740148D-04	1.61901710 05	1.59013610 04	-4.18778890 01	2.5C889120-07
REACTION CONSTANTS		'A'/'G'	'B'	'C'	'D'	'E'	'F'
		2.06598900 02 -2.55775050 03	-1.49789940-01	9.90575320 05	-1.55711920 04	-1.41132830 03	2.3101839D-04

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

10/31/73

BUNSENITE, HEAT OF FORMATION. BOYLE, KING, AND CONWAY, 1954.



THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2. THE SYSTEM AL-C AND THE THERMODYNAMICS OF BUNSENITE.

AT (A)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	5.979	6.618	1980.	172.	-0.1378	-0.0075	-153.
298.15	6.224	7.153	2133.	0.	0.0000	0.0000	0.
400.00	6.794	9.069	2798.	-830.	0.4532	0.0360	666.
500.00	7.379	10.643	3505.	-1817.	0.7942	0.0788	1372.
600.00	8.338	12.067	4287.	-2953.	1.0757	0.1281	2154.
700.00	9.787	13.454	5189.	-4229.	1.3204	0.1834	3056.
800.00	11.776	14.885	6262.	-5646.	1.5423	0.2448	4130.
900.00	14.327	16.413	7563.	-7209.	1.7567	0.3126	5430.
1000.00	17.454	18.080	9147.	-8933.	1.9523	0.3874	7014.
1100.00	21.163	19.912	11073.	-10831.	2.1519	0.4697	8940.
1200.00	25.458	21.934	13399.	-12922.	2.3533	0.5603	11266.
1300.00	30.342	24.160	16184.	-15224.	2.5555	0.6602	14051.
1400.00	35.818	26.606	19487.	-17761.	2.7726	0.7702	17355.
1500.00	41.885	29.280	23367.	-20553.	2.9946	0.8913	21235.
1600.00	48.545	32.193	27884.	-23625.	3.2270	1.0245	25751.
1700.00	55.798	35.351	33096.	-27000.	3.4711	1.1708	30964.
1800.00	63.646	38.759	39063.	-30703.	3.7279	1.3314	36931.
1900.00	72.087	42.424	45845.	-34760.	3.9984	1.5073	43712.
2000.00	81.123	46.349	53501.	-39197.	4.2832	1.6997	51368.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
1.37036280 01	-1.29019560-02	-2.16220390 05	-1.79449930 03	-6.5771C670 01	2.97703360-05	0.0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

NI (8)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	20.092	2.866	-5771.	-6554.	5.2442	0.2842	-464.
298.15	17.195	4.495	-5307.	-6647.	4.8725	0.2882	0.
400.00	10.910	8.513	-3930.	-7335.	4.0077	0.3181	1377.
500.00	8.581	10.657	-2973.	-8302.	3.6287	0.3600	2334.
600.00	7.685	12.129	-2167.	-9445.	3.4403	0.4096	3140.
700.00	7.423	13.289	-1415.	-10717.	3.3461	0.4647	3892.
800.00	7.460	14.280	-673.	-12097.	3.3047	0.5246	4634.
900.00	7.637	15.168	81.	-13570.	3.2953	0.5884	5388.
1000.00	7.869	15.984	856.	-15128.	3.3063	0.6560	6163.
1100.00	8.108	16.746	1655.	-16765.	3.3309	0.7270	6962.
1200.00	8.326	17.461	2477.	-18476.	3.3649	0.8012	7784.
1300.00	8.504	18.135	3319.	-20256.	3.4053	0.8784	8626.
1400.00	8.632	18.770	4176.	-22101.	3.4502	0.9584	9483.
1500.00	8.699	19.368	5043.	-24009.	3.4980	1.0411	10350.
1600.00	8.702	19.930	5914.	-25974.	3.5479	1.1263	11221.
1700.00	8.636	20.456	6781.	-27993.	3.5988	1.2139	12089.
1800.00	8.498	20.946	7639.	-30064.	3.6502	1.3037	12946.
1900.00	8.285	21.400	8479.	-32181.	3.7017	1.3955	13786.
2000.00	7.997	21.818	9293.	-34343.	3.7528	1.4892	14600.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
-3.10546950 00	6.81486260-03	1.47595590 06	0.0	2.66102410 01	-4.13146690-06	0.0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

BUNSENIT

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	10.024	8.178	-48119.	-50353.	40.2880	2.1835	-258.
298.15	10.566	9.080	-47862.	-50569.	37.0680	2.1928	0.
400.00	12.421	12.444	-46691.	-51669.	28.2306	2.2405	1170.
500.00	15.241	15.484	-45324.	-53066.	23.1950	2.3011	2578.
600.00	20.529	18.685	-43560.	-54771.	19.9504	2.3751	4302.
700.00	29.171	22.451	-41106.	-56822.	17.7405	2.4640	6756.
800.00	41.710	27.120	-37596.	-59292.	16.1977	2.5711	10266.
900.00	58.496	32.955	-32622.	-62285.	15.1248	2.7009	15240.
1000.00	79.763	40.182	-25747.	-65929.	14.4089	2.8589	22115.
1100.00	105.672	48.962	-16515.	-70373.	13.9818	3.0516	31347.
1200.00	136.342	59.437	-4454.	-75778.	13.8011	3.2860	43408.
1300.00	171.858	71.720	10915.	-82321.	13.8394	3.5657	58777.
1400.00	212.286	85.905	30081.	-90186.	14.0786	3.9108	77943.
1500.00	257.677	102.071	53538.	-99568.	14.5070	4.3176	101400.
1600.00	308.068	120.282	81783.	-110668.	15.1166	4.7985	129645.
1700.00	363.494	140.596	115319.	-123694.	15.9020	5.3638	163181.
1800.00	423.978	163.061	154651.	-138859.	16.8598	6.0214	202513.
1900.00	489.542	187.718	200284.	-156380.	17.9878	6.7811	248146.
2000.00	560.202	214.603	252729.	-176477.	19.2845	7.6526	300591.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
2.27006860 02	-1.62990600-01	8.55305780 05	-9.81501070 03	-1.49803820 03	2.60914170-04	-2.62571060 03

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2, THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

NIC (B)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS FN	LOG K	CELL EMF	HT2-HT1
273.15	13.725	7.289	-48384.	-50375.	40.3058	2.1844	-343.
298.15	13.725	8.491	-48041.	-50573.	37.0708	2.1930	0.
400.00	13.725	12.525	-46643.	-51653.	28.2219	2.2399	1398.
500.00	13.725	15.587	-45271.	-53064.	23.1944	2.3010	2770.
600.00	13.725	18.090	-43898.	-54752.	19.9434	2.3742	4143.
700.00	13.725	20.205	-42526.	-56669.	17.6930	2.4574	5515.
800.00	13.725	22.038	-41153.	-58784.	16.0589	2.5491	6888.
900.00	13.725	23.655	-39781.	-61070.	14.8298	2.6482	8260.
1000.00	13.725	25.101	-38408.	-63509.	13.8759	2.7540	9633.
1100.00	13.725	26.409	-37036.	-66085.	13.1300	2.8657	11005.
1200.00	13.725	27.603	-35663.	-68787.	12.5278	2.9828	12378.
1300.00	13.725	28.702	-34291.	-71603.	12.0375	3.1049	13750.
1400.00	13.725	29.719	-32918.	-74525.	11.6338	3.2316	15123.
1500.00	13.725	30.666	-31546.	-77544.	11.2982	3.3626	16495.
1600.00	13.725	31.551	-30173.	-80656.	11.0170	3.4975	17868.
1700.00	13.725	32.384	-28801.	-83853.	10.7800	3.6361	19240.
1800.00	13.725	33.168	-27428.	-87131.	10.5791	3.7783	20613.
1900.00	13.725	33.910	-26056.	-90485.	10.4081	3.9237	21985.
2000.00	13.725	34.614	-24683.	-93912.	10.2622	4.0723	23358.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
1.3724945D 01	0.0	0.0	-5.2133213D 04	-6.9707864D 01	0.0	0.0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

NIO (C)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	20.677	5.756	-48875.	-50447.	40.3629	2.1875	-495.
298.15	18.967	7.489	-48380.	-50613.	37.1003	2.1947	0.
400.00	15.156	12.441	-46673.	-51650.	28.2201	2.2397	1707.
500.00	13.639	15.636	-45244.	-53062.	23.1935	2.3010	3136.
600.00	12.981	18.056	-43918.	-54752.	19.9432	2.3742	4462.
700.00	12.729	20.035	-42635.	-56659.	17.6897	2.4569	5745.
800.00	12.694	21.731	-41365.	-58749.	16.0495	2.5476	7015.
900.00	12.785	23.230	-40092.	-60999.	14.8125	2.6451	8288.
1000.00	12.953	24.585	-38805.	-63390.	13.8540	2.7488	9575.
1100.00	13.173	25.830	-37499.	-65912.	13.0955	2.8582	10881.
1200.00	13.427	26.987	-36170.	-68553.	12.4853	2.9727	12210.
1300.00	13.706	28.072	-34813.	-71307.	11.9878	3.0921	13567.
1400.00	14.003	29.099	-33428.	-74166.	11.5778	3.2161	14952.
1500.00	14.312	30.075	-32012.	-77125.	11.2371	3.3444	16368.
1600.00	14.632	31.009	-30565.	-80180.	10.9520	3.4769	17815.
1700.00	14.960	31.906	-29085.	-83326.	10.7122	3.6133	19295.
1800.00	15.293	32.770	-27573.	-86560.	10.5098	3.7535	20807.
1900.00	15.631	33.606	-26027.	-89879.	10.3384	3.8974	22353.
2000.00	15.974	34.417	-24446.	-93280.	10.1932	4.0449	23934.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
8.46856410 00	1.82397740-03	8.36549800 05	-4.82612510 04	-3.7143274D 01	0.0	0.0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

(2 (C)

	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LOG K	CELL EMF	HT2-HT1
273.15	7.047	48.391	14436.	1218.	-0.9742	-0.0528	-176.
298.15	7.024	49.007	14611.	-0.	-0.0000	0.0000	-0.
400.00	7.187	51.088	15333.	-5102.	2.7876	0.2212	722.
500.00	7.443	52.719	16064.	-10295.	4.4959	0.4464	1453.
600.00	7.683	54.098	16821.	-15638.	5.6960	0.6781	2210.
700.00	7.888	55.298	17600.	-21109.	6.5904	0.9153	2989.
800.00	8.061	56.363	18398.	-26693.	7.2921	1.1575	3786.
900.00	8.206	57.321	19211.	-32378.	7.8623	1.4040	4600.
1000.00	8.328	58.192	20038.	-38154.	8.3385	1.6545	5427.
1100.00	8.434	58.991	20876.	-44013.	8.7447	1.9086	6265.
1200.00	8.525	59.728	21724.	-49950.	9.0971	2.1660	7113.
1300.00	8.605	60.414	22581.	-55957.	9.4073	2.4265	7969.
1400.00	8.678	61.055	23445.	-62031.	9.6835	2.6899	8834.
1500.00	8.743	61.655	24316.	-68167.	9.9319	2.9560	9705.
1600.00	8.804	62.222	25194.	-74361.	10.1573	3.2245	10582.
1700.00	8.862	62.757	26077.	-80610.	10.3632	3.4955	11466.
1800.00	8.917	63.265	26966.	-86912.	10.5525	3.7688	12355.
1900.00	8.971	63.749	27860.	-93263.	10.7276	4.0442	13249.
2000.00	9.024	64.210	28760.	-99661.	10.8904	4.3216	14149.

'A'	'B'	'C'	'D'	'E'	'F'	'G'
1.3406651D 01	-5.9740148D-04	1.61901710 05	1.59013610 04	-4.18778890 01	2.5088912D-07	-1.35920060 02

ATTACHMENT C

Listing of PHAS20 and Associated Routines

```
C     ------------------------------------------------------------------PHA  10
C                              PHAS20                                   PHA  20
C                                                                       PHA  30
C          THIS VERSION WILL HANOLE:                                    PHA  40
C                                                                       PHA  50
C                    20 PHASES                                          PHA  60
C                    70  OATA SETS                                      PHA  70
C                    ANO 1200 INDEPENOENT OBSERVATIONS.                 PHA  80
C                                                                       PHA  90
C          VERSION TESTEO  8/15/73 BY HAAS.                             PHA 100
C                                                                       PHA 110
C     ------------------------------------------------------------------PHA 120
      IMPLICIT REAL*8(A-H,O-Z)                                          PHA 130
      LOGICAL*1 LABEL,IMAGE,BCO                                         PHA 140
      REAL*4 XMAX,XMIN,YMAX,YMIN,XI,E,TITLE,ACOEF,T,TO,AVAL,RELERR,SERR,PHA 150
     1  SERRSQ,EBAR,STOEV,ERR,AN                                        PHA 160
      OIMENSION AVAL(7),SERR(3),SERRSQ(3),EBAR(3),STOEV(3),IMAGE(5000), PHA 170
     1  XI(1),E(1),PHINV(6),VAL(7),ION(20),IEMIN(20)                    PHA 180
      OIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),         PHA 190
     1  NPHASE(70),IKOUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),        PHA 200
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                          PHA 210
      OIMENSION X(2,1200),YO(1200),SIGYO(1200),P(140),KI(140),          PHA 220
     1  OC(140),PO(140),TITLE(20)                                       PHA 230
      OIMENSION REF(10,70),ERRP(140),IHOLO(40)                          PHA 240
      OIMENSION SCINV(2),STCOEF(10),YESNO(2),TK(19,2),TYPE(14),NSCALE(5)PHA 250
     1  ,LABEL(50)                                                      PHA 260
      OIMENSION OOOC(7),OYOC(7)                                         PHA 270
      OIMENSION AA(140)                                                 PHA 280
C     ------------------------------------------------------------------PHA 290
C         COMMON BLOCKS                                                 PHA 300
C            NAME             ROUTINES                                 PHA 310
C              EARTH            MAIN PROGRAM, ORGLS2, EAFW2O, PUTOUT    PHA 320
C              AIR              MAIN PROGRAM, ORGLS2, TEST2O, EAFW2O    PHA 330
C                               PUTOUT ANO UNIQUE.                      PHA 340
C              FIRE             MAIN PROGRAM, ORGLS2, TEST2O, EAFW2O    PHA 350
C              WATER            MAIN PROGRAM, EAFW2O, YOERIV, OOERIV,   PHA 360
C                               PUTOUT, FN, OIE, ANO PLOCK OATA.        PHA 370
C              TIME             MAIN PROGRAM, PUTOUT                    PHA 380
C              SPACE            MAIN PROGRAM, EAFW2O, YOERIV, OOERIV,   PHA 390
C                                  ANO PUTPUT                           PHA 400
C              MAN              MAIN PROGRAM, PUTOUT                    PHA 410
C     ------------------------------------------------------------------PHA 420
      COMMON /EARTH/ COEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGO,NSETS,    PHA 430
     1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                          PHA 440
      COMMON /AIR/ X, P, OC, TITLE, YO, SIGYO, PO, KI, NC, NV, NX, IW,  PHA 450
     1  NP, NO, ISING, ISTOP, IL, JN                                    PHA 460
      COMMON /FIRE/ REF, ERRP, IWRITE, ICY, IICY, IRECC, IREG, NHOLO,   PHA 470
     1 IHOLO                                                          PHA 480
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,             PHA 490
     1  SCINV, TREF, STCOEF, OIEO, AOIE, BOIE, THETA, YESNO, TK,        PHA 500
     2  ASTAR, TYPE, NL, NSCALE, LABEL, BCO                             PHA 510
      COMMON /TIME/ OATE                                                PHA 520
      COMMON /SPACE/ OOOC, OYOC, SC, TLOW                               PHA 530
      COMMON /MAN/ AA                                                   PHA 540
      EXTERNAL EAFW2O                                                   PHA 550
      CALL ERRSET (208,256,0,2)                                         PHA 560
C     ------------------------------------------------------------------PHA 570
C     READ IN AND STORE INPUT OATA--                                    PHA 580
C          OATE -- TOOAY'S OATE                                         PHA 590
C          NREG -- NUMBER OF SEPARATE PROBLEMS IN THE OATA SET          PHA 600
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C     ------------------------------------------------------------------PHA 610
      READ (5,4400) DATE                                                PHA 620
      READ (5,4500) NREG                                                PHA 630
      DO 4300 IREG=1,NREG                                               PHA 640
C     ------------------------------------------------------------------PHA 650
C     INITIALIZE CONSTANTS                                              PHA 660
C     WRITE DATE                                                        PHA 670
C     ------------------------------------------------------------------PHA 680
      IICY=0                                                            PHA 690
      KOUNT=0                                                           PHA 700
      IWRITE=1                                                          PHA 710
      WRITE (6,5300)                                                    PHA 720
      WRITE (6,5400) DATE                                               PHA 730
C     ------------------------------------------------------------------PHA 740
C     READ IN AND STORE --                                              PHA 750
C          TITLE (20) -- TITLE FOR CORRELATION                          PHA 760
C          IDO -- 1 FOR REGRESSION AND ERROR PLOTS                      PHA 770
C                 2 FOR REGRESSION ONLY                                 PHA 780
C                 3 FOR ERROR PLOTS ONLY                                PHA 790
C          NC -- NUMBER OF CYCLES. GENERALLY 2 IS SUFFICIENT.           PHA 800
C                SUBROUTINE TEST WILL TERMINATE REGRESSION              PHA 810
C                IF THE RELATIVE CHANGE IN SUCCESSIVE                   PHA 820
C                PARAMETERS IS LESS THAN THAN 1.00-8.                   PHA 830
C                                                                       PHA 840
C          IW -- 0 FOR WEIGHTED DATA                                    PHA 850
C                1 FOR UNWEIGHTED DATA                                  PHA 860
C          IL -- 0 FOR CALCULATED RESULTS AT PLOT TIME ONLY             PHA 870
C                1 FOR CALCULATED RESULTS WITH EACH CYCLE               PHA 880
C          IFMOUT -- PUNCH FORMAT FOR OUTPUT OF PARAMETERS--            PHA 890
C               0 GIVES PARAMETERS IN 6D12.5 FORMAT                     PHA 900
C               1 GIVES PARAMETERS IN 6A8 FORMAT.                       PHA 910
C          LISTP -- NUMBER OF PHASES IN CORRELATION                     PHA 920
C          ICY -- NUMBER OF STEPS IN STEP-BACKWARD ELIMINATION.         PHA 930
C               DEFAULT IS 0.                                           PHA 940
C          NHOLD -- NUMBER OF PARAMETERS TO BE KEPT WITHIN THE          PHA 950
C               REGRESSION EVEN THOUGH 'TEST' WILL INDICATE THEY ARE    PHA 960
C               NON-SIGNIFICANT.                                        PHA 970
C          PNAME(LISTP) -- 8-CHARACTER LABEL FOR EACH PHASE IN          PHA 980
C                          CORRELATION                                  PHA 990
C          ION(LISTP) -- FLAG WHICH INDICATES THE SPECIES IS A          PHA1000
C               REFERENCE ELEMENT (1), A COMPOUND (0), OR AN ION (-1).  PHA1010
C          NSETS -- NUMBER OF DATA SETS IN CORRELATION                  PHA1020
C     ------------------------------------------------------------------PHA1030
      READ (5,4600) (TITLE(I),I=1,20)                                   PHA1040
      READ (5,4500) IDO,NC,IW,IL,IFMOUT                                 PHA1050
      READ (5,4500) LISTP,ICY,NHOLD                                     PHA1060
      READ (5,4400) (PNAME(M),M=1,LISTP)                                PHA1070
      READ (5,4700) (ION(I),I=1,LISTP)                                  PHA1080
      READ (5,4500) NSETS                                               PHA1090
      WRITE (6,5500) (TITLE(I),I=1,20)                                  PHA1100
      WRITE (6,5600) (PNAME(M),M=1,LISTP)                               PHA1110
      WRITE (6,5300)                                                    PHA1120
      WRITE (6,5700) (TITLE(I),I=1,20),DATE                             PHA1130
      WRITE (6,5800)                                                    PHA1140
      PUNCH 4600, (TITLE(I),I=1,20)                                     PHA1150
      PUNCH 4500, LISTP                                                 PHA1160
      PUNCH 4400, (PNAME(M),M=1,LISTP)                                  PHA1170
C     ------------------------------------------------------------------PHA1180
C     READ IN AND STORE INPUT DATA FOR EACH DATA SET --                 PHA1190
C          REF (10,J) -- REFERENCE FOR 'J'TH DATA SET (DATA SET         PHA1200
C                        IDENTIFICATION)                                PHA1210
C          NPHASE(J) -- NUMBER OF PHASES IN REACTION, SET TO 1 WHEN
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C                        DATA FOR ONE PHASE ONLY.                          PHA1220
C          IKOUNT(J) -- NUMBER OF OBSERVATIONS IN DATA SET                 PHA1230
C          IGO(J) -- DATA TYPE,                                            PHA1240
C                        FOR HEAT CAPACITY, IGO(J) IS  1                   PHA1250
C                            ENTROPY                   2                   PHA1260
C                            ENTHALPY                  3                   PHA1270
C                            GIBBS ENERGY              4                   PHA1280
C                            LOG(10) K                 5                   PHA1290
C                            CELL DATA                 6                   PHA1300
C                            DIFFERENTIAL HEAT,                            PHA1310
C                               H(T)-H(TO)             7                   PHA1320
C                        FOR ANY DATA NOT INCLUDED IN TYPES 1              PHA1330
C                          THROUGH 7, SET IGO(J) TO ANY INTEGER            PHA1340
C                          8 THRU 14.  SUPPLY SUBROUTINE UNIQUE            PHA1350
C                          TO CALCULATE YC (AND THE DERIVATIVES            PHA1360
C                          DC(I) IF JN (OR JDFLAG) = ZERO) FROM            PHA1370
C                          THE  CURRENT VALUES OF THE PARAMETERS.          PHA1380
C                          IF MORE THAN ONE TYPE OF DATA ARE TO BE         PHA1390
C                          CONSIDERED, THESE ARE KEYED BY DIFFERENT        PHA1400
C                          VALUES OF IGO(J).                               PHA1410
C          ITEMP -- THE VALUES IS 1 IF TEMPERATURE IS IN KELVINS,          PHA1420
C               0 IF THE TEMPERATURE IS IN CENTIGRADE DEGREES.             PHA1430
C          IPARA -- PROGRAM IS SET FOR UNITS IN JOULES(*), VOLTS, OR       PHA1440
C               LOG(10)K IN MOLAL UNITS.                                   PHA1450
C               IF SO, SET IPARA TO 1                                      PHA1460
C               IF NOT, SET IPARA TO 0.  PROGRAM MULTIPLIES YO(I) AND      PHA1470
C               SIGYO(I)BY PARA TO BE READ LATER.                          PHA1480
C          ISIG -- 0 IF WEIGHTS ARE RELATIVE.                              PHA1490
C               1 IF WEIGHTS ARE ABSOLUTE.                                 PHA1500
C               (ABSOLUTE WEIGHTS ARE USED IN CALCULATIONS.)               PHA1510
C                                                                          PHA1520
C     (*)  FOR DATA IN CALORIES, ADJUST R AND F IN BLOCK DATA.  SEE        PHA1530
C          COMMENTS IN BLOCK DATA WHICH DESCRIBE THE NECESSARY             PHA1540
C          ADJUSTMENTS.                                                    PHA1550
C                                                                          PHA1560
C     ------------------------------------------------------------------PHA1570
      DO 1800 J=1,NSETS                                                    PHA1580
      READ (5,4400) (REF(I,J),I=1,10)                                      PHA1590
      WRITE (6,5900)                                                       PHA1600
      WRITE (6,6000) ASTAR                                                 PHA1610
      WRITE (6,5900)                                                       PHA1620
      WRITE (6,6100) J,(REF(I,J),I=1,10)                                   PHA1630
      READ (5,4500) NPHASE(J),IKOUNT(J),IGO(J),ITEMP,IPARA,ISIG            PHA1640
      WRITE (6,6200) NPHASE(J),IKOUNT(J),TYPE(IGO(J))                      PHA1650
      NPHAS=NPHASE(J)                                                      PHA1660
C     ------------------------------------------------------------------PHA1670
C     FOR EACH DATA SET, READ AND STORE FOR ONE PHASE AT A TIME,           PHA1680
C          ANAME -- 8-CHARACTER PHASE LABEL. MUST BE THE SAME AS           PHA1690
C                        GIVEN IN PNAME(LISTP).                            PHA1700
C          COEF(I,J) -- COEFFICIENT IN REACTION (+1.0D0 IF NOT             PHA1710
C                        REACTION)                                         PHA1720
C          ISTATE(I,J) -- FOR ELEMENTS IN LOWEST TEMPERATURE MODIFICA-     PHA1730
C                        TION, SET TO 1                                    PHA1740
C                       FOR COMPOUNDS AND ELEMENTS IN HIGHER TEMPER-PHA1750
C                        ATURE MODIFICATIONS, SET TO 0                     PHA1760
C          NINVER(I,J) -- NUMBER OF INVERSIONS(EQUALS NUMBER OF LOWER      PHA1770
C                        TEMPERATURE MODIFICATIONS BEING CONSIDERED PHA1780
C                        FOR COMPONENT.)                                   PHA1790
C     ------------------------------------------------------------------PHA1800
      DO 700 I=1,NPHAS                                                     PHA1810
      READ (5,4800) ANAME,COEF(I,J),ISTATE(I,J),NINVER(I,J)                PHA1820
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C     ------------------------------------------------------------------PHA1830
C     LOCATE ANAME IN LIST  PNAME(LISTP) AND ASIGN THE INDEX TO          PHA1840
C          IPHASE(I,J).                                                  PHA1850
C     ------------------------------------------------------------------PHA1860
      DO 100 K=1,LISTP                                                   PHA1870
      IF (ANAME.EQ.PNAME(K)) GO TO 200                                   PHA1880
  100 CONTINUE                                                           PHA1890
      GO TO 4100                                                         PHA1900
  200 IPHASE(I,J)=K                                                      PHA1910
      NOYES=(ISTAT(I,J)+3)/2                                             PHA1920
      ACOEF=COEF(I,J)                                                    PHA1930
      WRITE (6,6300) PNAME(IPHASE(I,J)),ACOEF,YESNO(NOYES),NINVER(I,J)   PHA1940
      IF (NINVER(I,J).EQ.0) GO TO 700                                    PHA1950
C     ------------------------------------------------------------------PHA1960
C     IF (NINVER(I,J).GT.0) READ AND STORE,                              PHA1970
C          INSTAT(I,J) -- FOR ELEMENTS,ASIGN 1                           PHA1980
C                         FOR COMPOUNDS, ASIGN 0                         PHA1990
C          INVSC(I,J) -- IF UPON INVERSION THERE IS A STOICHIOMETRY      PHA2000
C               CHANGE (EG-- 2 FECL3 = FE2CL6), THEN FIND THE APPRO-     PHA2010
C               PRIATE REACTANT COEFFICIENT (HERE '2') IN THE VECTOR     PHA2020
C               STCOEF AND ENTER HERE.  DEFAULT GIVES A COEFFICIENT OF   PHA2030
C               '1'.                                                     PHA2040
C          TINV(NINVER(I,J)) -- INVERSION TEMPERATURES, KELVINS          PHA2050
C          PHINV(NINVER(I,J)+1) -- PHASE NAME FOR ALL MODIFICATIONS,     PHA2060
C                         BEGINNING WITH LOWEST TEMPERATURE MODIFICA-    PHA2070
C                         TION FIRST. NAME MUST CONFORM WITH NAMES       PHA2080
C                         IN PNAME(LISTP).                               PHA2090
C     ------------------------------------------------------------------PHA2100
      KINVER=NINVER(I,J)                                                 PHA2110
      READ (5,4900) (TINV(I,J,K),K=1,KINVER)                             PHA2120
      KINVER=KINVER+1                                                    PHA2130
      READ (5,5000) INSTAT(I,J),INVSC(I,J),(PHINV(K),K=1,KINVER)         PHA2140
      IF (INVSC(I,J).EQ.0) INVSC(I,J)=1                                  PHA2150
C     ------------------------------------------------------------------PHA2160
C     LOCATE PHINV(NINVER(I,J)+1) IN LIST PNAME(LISTP) AND ASIGN THE     PHA2170
C          INDEX TO INVPH(I,J).                                          PHA2180
C     ------------------------------------------------------------------PHA2190
      DO 500 K=1,KINVER                                                  PHA2200
      DO 300 L=1,LISTP                                                   PHA2210
      IF (PHINV(K).EQ.PNAME(L)) GO TO 400                                PHA2220
  300 CONTINUE                                                           PHA2230
      GO TO 4100                                                         PHA2240
  400 INVPH(I,J,K)=L                                                     PHA2250
  500 CONTINUE                                                           PHA2260
      KINVER=KINVER-1                                                    PHA2270
      WRITE (6,6400)                                                     PHA2280
      ACOEF=1.0                                                          PHA2290
      DO 600 K=1,KINVER                                                  PHA2300
      IF (K.EQ.KINVER) ACOEF=STCOEF(INVSC(I,J))                          PHA2310
      T=TINV(I,J,K)                                                      PHA2320
      WRITE (6,6500) ACOEF,PNAME(INVPH(I,J,K)),PNAME(INVPH(I,J,K+1)),T   PHA2330
  600 CONTINUE                                                           PHA2340
      IF (INSTAT(I,J).EQ.1) WRITE (6,6600) PNAME(INVPH(I,J,1))           PHA2350
  700 CONTINUE                                                           PHA2360
C     ------------------------------------------------------------------PHA2370
C     INITIALIZE KO, KCUNT,AND IKOUNT(I). AFTER DATA IS STORED,          PHA2380
C          IKOUNT(I) CONTAINS THE LOCATION OF THE LAST ITEM IN THE       PHA2390
C          'J'TH DATA SET.                                               PHA2400
C     ------------------------------------------------------------------PHA2410
      KO=KCUNT+1                                                         PHA2420
      KCUNT=KOUNT+IKOUNT(J)                                              PHA2430
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      IKCUNT(J)=KCUNT                                                   PHA2440
      WRITE (6,6700)                                                    PHA2450
      WRITE (6,6800) TYPE(IGO(J))                                       PHA2460
C     ------------------------------------------------------------------PHA2470
C     READ AND STORE THE DATA (N THE 'J'TH DATA SET,                    PHA2480
C          X(1,I) -- TEMPERATURE (SEE TFACT BELOW)                      PHA2490
C          TFACT -- 0.0D0 IF TEMPERATURE IN KELVINS                     PHA2500
C                   273.1500 IF TEMPERATURE IN CENTIGRADE DEGREES       PHA2510
C          YO(I)  -- DEPENDANT OBSERVATION                              PHA2520
C          PARA -- CONVERSION FACTOR TO CONVERT DATA TO CALORIES OR     PHA2530
C                       VOLTS  (1.0D3 FOR DATA IN KILOCALORIES,         PHA2540
C                       1.0D-3 FOR DATA IN MILLIVOLTS, --OR THE         PHA2550
C                       APPROPIATE CONVERSION FACTOR FOR DATA IN        PHA2560
C                       JOULES, BTU/LB,  QUART*STONES/ACRE,ETC.)        PHA2570
C          SIGYC(I)  -- SEE PROGRAM DESCRIPTION FOR ASIGNING WEIGHTS.   PHA2580
C          X(2,I) -- FOR DATA TYPES (IGO(J)) FROM 1 THRU 6,             PHA2590
C                       X(2,I) = ZERO.                                  PHA2600
C                    FOR RELATIVE HEAT CONTENT DATA, X(2,I) IS THE BASE PHA2610
C                       TEMPERATURE.   DEFAULT IS 298.15 K.             PHA2620
C                    FOR DATA TYPES TO BE PROGRAMMED BY THE USER,       PHA2630
C                       X(2,I) IS AN OPTIONAL SECOND INDEPENDENT        PHA2640
C                       VARIABLE.                                       PHA2650
C     ------------------------------------------------------------------PHA2660
      DO 1700 I=KO,KOUNT                                                PHA2670
      READ (5,4900) X(1,I),TFACT,YO(I),PARA,SIGYC(I),X(2,I)             PHA2680
      IF ((IW.EQ.0).AND.(SIGYO(I).EQ.0.0D0).AND.(ISIG.EQ.0)) SIGYC(I)=(.PHA2690
     1DO                                                                PHA2700
      IF (ITFACT.EQ.1) GO TO 1000                                       PHA2710
C     ------------------------------------------------------------------PHA2720
C          IF (TFACT = 0     X(1,I) = X(1,I) + TFACT                    PHA2730
C     ------------------------------------------------------------------PHA2740
      X(1,I)=X(1,I)+TFACT                                               PHA2750
      IF (IGO(J).EQ.7) GO TO 800                                        PHA2760
      X(2,I)=0.0D0                                                      PHA2770
      GO TO 900                                                         PHA2780
  800 X(2,I)=X(2,I)+TFACT                                               PHA2790
  900 CONTINUE                                                          PHA2800
 1000 CONTINUE                                                          PHA2810
      IF (IPARA.EQ.1) GO TO 1100                                        PHA2820
C     ------------------------------------------------------------------PHA2830
C     IF IPARA = 0      YO(I) = YO(I)*PARA                              PHA2840
C     ------------------------------------------------------------------PHA2850
      YO(I)=YO(I)*PARA                                                  PHA2860
 1100 CONTINUE                                                          PHA2870
      IF (IW.EQ.1) GO TO 1300                                           PHA2880
      IF (ISIG.EQ.1) GO TO 1200                                         PHA2890
C     ------------------------------------------------------------------PHA2900
C     IF ISIG = 0         SIGYO(I)= DABS (YO(I))*S(GYO(I)               PHA2910
C     ------------------------------------------------------------------PHA2920
      SIGYO(I)=DABS(SIGYO(I)*YO(I))                                     PHA2930
      GO TO 1400                                                        PHA2940
 1200 CONTINUE                                                          PHA2950
C     ------------------------------------------------------------------PHA2960
C     IF IPARA = 0       SIGYO(I)=SIGYO(I)*PARA                         PHA2970
C     ------------------------------------------------------------------PHA2980
      IF (IPARA.EQ.0) SIGYO(I)=DABS(SIGYO(I)*PARA)                      PHA2990
      GO TO 1400                                                        PHA3000
 1300 CONTINUE                                                          PHA3010
      SIGYC(I)=DABS(YO(I)*1.0D-2)                                       PHA3020
 1400 CONTINUE                                                          PHA3030
      IF (SIGYO(I).EQ.0.0D0) SIGYO(I)=1.0D0                             PHA3040
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      IF (IIIGO(J).EQ.7).AND.(X(2,I).EQ.0.0D0)) X(2,I)=298.1500          PHA3050
      T=X(1,I)                                                           PHA3060
      TC=X(2,I)                                                          PHA3070
      IF (TO.NE.0.0) GO TO 1500                                          PHA3080
      WRITE (6,6900) I,T,Y0(I),SIGY0(I)                                  PHA3090
      GO TO 1600                                                         PHA3100
 1500 CONTINUE                                                           PHA3110
      WRITE (6,7000) I,T,TO,Y0(I),SIGY0(I)                               PHA3120
 1600 CONTINUE                                                           PHA3130
 1700 CONTINUE                                                           PHA3140
 1800 CONTINUE                                                           PHA3150
      WRITE (6,7100) (J,IKOUNT(J),J=1,NSETS)                             PHA3160
C     ------------------------------------------------------------------PHA3170
C     THE DATA HAS NOW BEEN STORED. INITIALIZE CONSTANTS NEEDED FOR      PHA3180
C          ORGLS2.                                                       PHA3190
C     ------------------------------------------------------------------PHA3200
      NC=KCUNT                                                           PHA3210
      NP=LISTP*7                                                         PHA3220
      NX=2                                                               PHA3230
      I=0                                                                PHA3240
C     ------------------------------------------------------------------PHA3250
C     READ AND STORE,                                                    PHA3260
C          IFMIN -- INPUT FORMAT CDE PILISTP*7)                          PHA3270
C               0 INDICATES (6D12.5/D12.5)                             PHA3280
C               1 INDICATES (7A8)                                      PHA3290
C               THE LATTER FORMAT HAS NO ROUNDOFF IN DATA TRANSFER.    PHA3300
C     PILISTP*6)  -- TRIAL PARAMETERS. IF VARIED, MAY NOT BE 0.0D0       PHA3310
C                                    IF NOT VARIED, 0.0D0 OR A         PHA3320
C                                    PREDETERMINED VALUE MAY BE USED   PHA3330
C     KIILISTP*6)  -- 0 IF PARAMETER IS HELD CONSTANT.                   PHA3340
C                     1 IF PARAMETER IS TO BE VARIED                   PHA3350
C          IHOLD -- INDICES OF PARAMETERS IN PILISTP*7) WHICH ARE       PHA3360
C               FORCED TO STAY IN REGRESSION DESPITE 'TEST' DETERMINA-  PHA3370
C               TION THAT THESE PARAMETERS MAY BE NON-SIGNIFICANT.      PHA3380
C     ------------------------------------------------------------------PHA3390
      READ (5,5100) (IFMIN(I),I=1,LISTP)                                PHA3400
      DO 2100 I=1,LISTP                                                  PHA3410
      JO=1+7*(I-1)                                                       PHA3420
      JN=JO+6                                                            PHA3430
      IF (IFMIN(I).EQ.1) GO TO 1900                                      PHA3440
      READ (5,4900) (P(J),J=JO,JN)                                       PHA3450
      GO TO 2000                                                         PHA3460
 1900 CONTINUE                                                           PHA3470
      READ (5,4400) (P(J),J=JO,JN)                                       PHA3480
 2000 CONTINUE                                                           PHA3490
      DO 2100 J=JO,JN                                                    PHA3500
      A(J)=P(J)                                                          PHA3510
 2100 CONTINUE                                                           PHA3520
      READ (5,5100) (KI(I),I=1,NP)                                       PHA3530
      IF (NHOLD.NE.0) READ (5,4700) (IHOLD(I),I=1,NHOLD)                 PHA3540
C     ------------------------------------------------------------------PHA3550
C     BYPASS REGRESSION IF IDC IS 3.                                     PHA3560
C     ------------------------------------------------------------------PHA3570
      IF (IDD.EQ.3) GO TO 2600                                           PHA3580
 2200 CONTINUE                                                           PHA3590
      NV=0                                                               PHA3600
      DO 2300 K=1,NP                                                     PHA3610
      IF (KI(K).EQ.0) GO TO 2300                                         PHA3620
      NV=NV+1                                                            PHA3630
 2300 CONTINUE                                                           PHA3640
      JN=0                                                               PHA3650
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C     ------------------------------------------------------------------PHA3660
C     ENTER DRGLS2 AND REFINE PARAMETERS                                PHA3670
C     ------------------------------------------------------------------PHA3680
      CALL DRGLS2 (EAFW20)                                              PHA3690
      IF (ISING.NE.0) GO TO 2600                                        PHA3700
C     ------------------------------------------------------------------PHA3710
C     PUNCH REFINED PARAMETERS ON CARD, ONE PHASE AT A TIME AND INCLUDE PHA3720
C          THE PHASE NAME ON THE CARD WITH THE RELATED PARAMETERS.      PHA3730
C     ------------------------------------------------------------------PHA3740
      DO 2500 I=1,LISTP                                                 PHA3750
      JC=1+7*(I-1)                                                      PHA3760
      IF (IFMOUT.EQ.1) GO TO 2400                                       PHA3770
      JN=JC+5                                                           PHA3780
      PUNCH 820C, (P(J),J=JC,JN),PNAME(I)                               PHA3790
      JN=JN+1                                                           PHA3800
      PUNCH 830C, P(JN),DATE,PNAME(I)                                   PHA3810
      GO TO 2500                                                        PHA3820
 2400 CONTINUE                                                          PHA3830
      JN=JC+6                                                           PHA3840
      PUNCH 840C, (P(J),J=JC,JN),DATE,PNAME(I)                          PHA3850
 2500 CONTINUE                                                          PHA3860
      IF (IDO.EC.2) GO TO 4000                                          PHA3870
 2600 CONTINUE                                                          PHA3880
      IF (IICY.GE.1) GO TO 2700                                         PHA3890
C     ------------------------------------------------------------------PHA3900
C     SET UP AND PRINT ERROR PLOTS.                                     PHA3910
C     READ IN AND STORE                                                 PHA3920
C          NHL -- NUMBER OF HORIZONTAL DIVISIONS ON ORDINATE LESS 1.    PHA3930
C          NSBH -- NUMBER OF HORIZONTAL LINES PER DIVISION.             PHA3940
C          NVL -- NUMBER OF VERTICAL DIVISIONS ON ABSCISSA LESS 1.      PHA3950
C          NSBV -- NUMBER OF VERTICAL LINES PER DIVISION.               PHA3960
C          XMAX -- MAXIMUM TEMPERATURE ON ABSCISSA.                     PHA3970
C          XMIN -- MINIMUM TEMPERATURE ON ABSCISSA.                     PHA3980
C          YMAX -- MAXIMUM ERROR ON ORDINATE.                           PHA3990
C               YMIN = - YMAX.                                          PHA4000
C     ------------------------------------------------------------------PHA4010
      READ (5,4500) NHL,NSBH,NVL,NSBV                                   PHA4020
      READ (5,5200) XMAX,XMIN,YMAX                                      PHA4030
      YMIN=-YMAX                                                        PHA4040
 2700 CONTINUE                                                          PHA4050
      IF ((ISING.NE.0).AND.(IDO.NE.3)) GO TO 4200                       PHA4060
      IN=0                                                              PHA4070
      DO 3300 J=1,NSETS                                                 PHA4080
      WRITE (6,5300)                                                    PHA4090
      WRITE (6,5700) (TITLE(I),I=1,20),DATE                             PHA4100
      WRITE (6,7200) TYPE(IGO(J))                                       PHA4110
C     ------------------------------------------------------------------PHA4120
C     INITIALIZE THE PLOT IMAGE.                                        PHA4130
C     ------------------------------------------------------------------PHA4140
      CALL PLOTI (NSCALE,NHL,NSBH,NVL,NSBV)                             PHA4150
      CALL PLOT2 (IMAGE,XMAX,XMIN,YMAX,YMIN)                            PHA4160
C     ------------------------------------------------------------------PHA4170
C     INITIALIZE CONSTANTS AND COUNTERS.                                PHA4180
C     ------------------------------------------------------------------PHA4190
      IC=IN+1                                                           PHA4200
      IN=IKOUNT(J)                                                      PHA4210
      DO 2800 I=1,3                                                     PHA4220
      SERR(I)=ZERO                                                      PHA4230
      SERRSQ(I)=ZERO                                                    PHA4240
 2800 CONTINUE                                                          PHA4250
C     ------------------------------------------------------------------PHA4260
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C      CALCULATE AND PRINT YC.  CALCULATE AND SUM THE DIFFERENCE (ERR),  PHA4270
C        PERCENT ERROR (RELERR), AND THE WEIGHTED DIFFERENCE (E).        PHA4280
C     ------------------------------------------------------------------PHA4290
      DO 3100 I=IO,IN                                                    PHA4300
      CALL EAFW20 (YC,I)                                                 PHA4310
      ERROP=YO(I)-YC                                                     PHA4320
      ERR=ERROP                                                          PHA4330
      IF (YO(I).EQ.ZERO) GO TO 2900                                      PHA4340
      RELERR=ERROP*1.0D2/DABS(YO(I))                                     PHA4350
      GO TO 3000                                                         PHA4360
 2900 CONTINUE                                                           PHA4370
      RELERR=ZERO                                                        PHA4380
 3000 CONTINUE                                                           PHA4390
      E(I)=ERR/SIGYO(I)                                                  PHA4400
      XI(I)=X(1,I)                                                       PHA4410
      TC=X(2,I)                                                          PHA4420
      WRITE (6,7300) XI(I),TC,YO(I),YC,ERR,RELERR,E(I)                   PHA4430
C     ------------------------------------------------------------------PHA4440
C     ENTER THE POINT ON THE PLOT IMAGE.                                 PHA4450
C     SUM THE ERRORS.                                                    PHA4460
C     ------------------------------------------------------------------PHA4470
      CALL PLOT3 (BCD,XI,E,1)                                            PHA4480
      SERR(1)=SERR(1)+ERR                                                PHA4490
      SERR(2)=SERR(2)+RELERR                                             PHA4500
      SERR(3)=SERR(3)+E(I)                                               PHA4510
      SERRSQ(1)=SERRSQ(1)+ERR*ERR                                        PHA4520
      SERRSQ(2)=SERRSQ(2)+RELERR*RELERR                                  PHA4530
      SERRSQ(3)=SERRSQ(3)+E(I)*E(I)                                      PHA4540
C     ------------------------------------------------------------------PHA4550
C     CALCULATE AND WRITE THE STANDARD ERROR OF ESTIMATE FOR THE         PHA4560
C        DIFFERENCE, THE PERCENT ERROR, AND THE WEIGHTED DIFFERENCE.     PHA4570
C     ------------------------------------------------------------------PHA4580
 3100 CONTINUE                                                           PHA4590
      NDATA=1+(IN-IO)                                                    PHA4600
      AN=NDATA                                                           PHA4610
      DO 3200 I=1,3                                                      PHA4620
      EBAR(I)=SERR(I)/AN                                                 PHA4630
      STDEV(I)=SQRT(SERRSQ(I)/AN-EBAR(I)*EBAR(I))                        PHA4640
 3200 CONTINUE                                                           PHA4650
      WRITE (6,7700)                                                     PHA4660
      WRITE (6,7400) (EBAR(I),I=1,3),(STDEV(I),I=1,3),NDATA              PHA4670
C     ------------------------------------------------------------------PHA4680
C     CALL PUTOLT TO CALCULATE AND WRITE THE COMPLETE SET OF CONSTANTS   PHA4690
C        FOR THE PHASES AND FOR THE DATA SET.  BYPASS THE LATTER SET     PHA4700
C        OF CONSTANTS IF IGO(J) IS GREATER THAN OR EQUAL TO 7 OR IF      PHA4710
C        THE J-TH DATA SET HAS ONLY ONE PHASE.                           PHA4720
C     ------------------------------------------------------------------PHA4730
      CALL PUTOLT (J)                                                    PHA4740
C     ------------------------------------------------------------------P.A4750
C      PRINT THE PLOT IMAGE FOR THE J-TH DATA SET.                       PHA4760
C     ------------------------------------------------------------------PHA4770
      WRITE (6,5300)                                                     PHA4780
      WRITE (6,5700) (TITLE(I),I=1,20),DATE                              PHA4790
      WRITE (6,7500) (REF(I,J),I=1,10)                                   PHA4800
      CALL PLOT4 (NL,LABEL)                                              PHA4810
      WRITE (6,7600)                                                     PHA4820
 3300 CONTINUE                                                           PHA4830
C     ------------------------------------------------------------------PHA4840
C     PUT OUT TABLES FOR EACH SPECIES IN THE LIST PNAME(LISTP).          PHA4850
C     ------------------------------------------------------------------PHA4860
      SC=1.0D0                                                           PHA4870
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      DO 3900 L=1,LISTP                                                 PHA4880
      WRITE (6,5400) DATE                                               PHA4890
      WRITE (6,5500) (TITLE(I),I=1,20)                                  PHA4900
      WRITE (6,7700) PNAME(L)                                           PHA4910
      WRITE (6,7800) (TYPE(I),I=1,7)                                    PHA4920
      INDEX=1+7*(L-1)                                                   PHA4930
      KOUNT=19                                                          PHA4940
      IF (IDN(L).EQ.-1) KOUNT=15                                        PHA4950
      M=(ICN(L)+4)/2                                                    PHA4960
      DO 3800 K=1,KOUNT                                                 PHA4970
      T=TK(K,M)                                                         PHA4980
      DO 3600 J=1,7                                                     PHA4990
      VAL(J)=0.000                                                      PHA5000
      IGOES=J                                                           PHA5010
      IF (IDN(L).EQ.-I) IGOES=IGOES+7                                   PHA5020
      IF (IGOES.EQ.14) GO TO 3600                                       PHA5030
      CALL YDERIV (TK(K,M),IGOES)                                       PHA5040
      DO 3400 I=1,7                                                     PHA5050
      VAL(J)=VAL(J)+OYDC(I)*AA(INDEX+I-1)                               PHA5060
 3400 CONTINUE                                                          PHA5070
      IF (J.NE.7) GO TO 3600                                            PHA5080
      CALL YDERIV (298.15D0,J)                                          PHA5090
      DO 3500 I=1,7                                                     PHA5100
      VAL(J)=VAL(J)-OYDC(I)*AA(INDEX+I-1)                               PHA5110
 3500 CONTINUE                                                          PHA5120
 3600 CONTINUE                                                          PHA5130
      DO 3700 I=1,7                                                     PHA5140
      AVAL(I)=VAL(I)                                                    PHA5150
 3700 CONTINUE                                                          PHA5160
      WRITE (6,7900) T,(AVAL(I),I=1,7)                                  PHA5170
 3800 CONTINUE                                                          PHA5180
      JO=INDEX                                                          PHA5190
      JN=JO+6                                                           PHA5200
      WRITE (6,8700)                                                    PHA5210
      WRITE (6,8000) (AA(J),J=JO,JN)                                    PHA5220
      PUNCH 8500, (AA(J),J=JO,JN),PNAME(L),DATE                         PHA5230
 3900 CONTINUE                                                          PHA5240
      IF (IDJ.EQ.3) GO TO 4200                                          PHA5250
C     ------------------------------------------------------------------PHA5260
C     IF STEP-BACKWARD ELIMINATION OF NON-SIGNIFICANT PARAMETERS IS     PHA5270
C          IN EFFECT (ICY.NE.0), SET LEAST SIGNIFICANT PARAMETER TO     PHA5280
C          ZERO AND REPEAT REGRESSION.                                  PHA5290
C     ------------------------------------------------------------------PHA5300
 4000 IF ((IREDC.EQ.0).OR.(IICY.GT.ICY)) GO TO 4200                     PHA5310
      KI(IREDO)=0                                                       PHA5320
      P(IREDO)=C.000                                                    PHA5330
      IICY=IICY+1                                                       PHA5340
      GO TO 2200                                                        PHA5350
 4100 CONTINUE                                                          PHA5360
      WRITE (6,8100) J                                                  PHA5370
 4200 CONTINUE                                                          PHA5380
 4300 CONTINUE                                                          PHA5390
      STOP                                                              PHA5400
C     ------------------------------------------------------------------PHA5410
C     FORMAT STATEMENTS                                                 PHA5420
C     ------------------------------------------------------------------PHA5430
 4400 FORMAT (1CA8)                                                     PHA5440
 4500 FORMAT (16I5)                                                     PHA5450
 4600 FORMAT (2CA4)                                                     PHA5460
 4700 FORMAT (4CI2)                                                     PHA5470
 4800 FORMAT (A8,2X,D10.3,10X,2I5)                                      PHA5480
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 4900 FORMAT (6D12.5)                                                    PHA5490
 5000 FORMAT (I5,13,9A8/(10A8))                                          PHA5500
 5100 FORMAT (8D11)                                                      PHA5510
 5200 FORMAT (8E10.3)                                                    PHA5520
 5300 FORMAT (1H1)                                                       PHA5530
 5400 FORMAT (42H1 THESE RESULTS WERE OBTAINED IN A RUN ON ,A8)          PHA5540
 5500 FORMAT (1H0,20A4/1H0)                                              PHA5550
 5600 FORMAT (6CH0     PHASES CONSIDERED IN THIS REGRESSION ARE AS FOLLOPHA5560
     1WS---/1H0,10X,5A2C/(1H ,10X,5A20))                                 PHA5570
 5700 FORMAT (1H ,20A4,40X,A8/1H0)                                       PHA5580
 5800 FORMAT (54H0THE FOLLOWING DATA SETS HAVE BEEN READ IN TO STORAGE:/PHA5590
     111H0SET NUMBER,10X,9HREFERENCE)                                    PHA5600
 5900 FORMAT (1H0)                                                       PHA5610
 6000 FORMAT (1H ,A8)                                                    PHA5620
 6100 FORMAT (1H ,I6,14X,10A8)                                           PHA5630
 6200 FORMAT (25H0THE NUMBER OF PHASES IS:,I5/31H THE NUMBER OF OBSERVATPHA5640
     1IONS IS:,I5/21H THE TYPE OF DATA IS:,3X,A8/11H0PHASE NAME,10X,11HCPHA5650
     20EFFICIENT,9X,10HREF. STATE,10X,10HINVERSIONS/1H )                 PHA5660
 6300 FORMAT (1H ,1X,A8,11X,F8.3,15X,A3,14X,I6)                          PHA5670
 6400 FORMAT (1H0,10X,26HINVERSIONS ARE AS FOLLOWS:/1H )                 PHA5680
 6500 FORMAT (1H ,F15.2,3X,A8,5X,1H=,5X,A8,F20.3)                        PHA5690
 6600 FORMAT (1H0,10X,A8,5X,58HIS A REFERENCE PHASE AND HAS ZERO GIBBS EPHA5700
     1NERGY AT 298.15 K/1H0)                                             PHA5710
 6700 FORMAT (1H )                                                       PHA5720
 6800 FORMAT (1H ,15X,5HINDEX,21X,11HTEMPERATURE,18X,A8,13X,5HERROR/1H ,PHA5730
     135X,2HT2,18X,2HT1/1H )                                             PHA5740
 6900 FORMAT (1H ,I20,F20.3,16X,1H-,3X,1P2D20.5)                         PHA5750
 7000 FORMAT (1H ,I20,2F20.3,1P2D20.5)                                   PHA5760
 7100 FORMAT (93H1THE INDEX OF THE LAST ITEM OF THE ABOVE DATA SETS IN TPHA5770
     1HE VECTORS X(1,I), YO(I), AND SIGYO(I)/15H IS AS FOLLOWS:/1H0,30X,PHA5780
     28HDATA SET,3X,5H1NDEX//(1H ,24X,2I10))                             PHA5790
 7200 FORMAT (1H ,9X,11HTEMPERATURE,20X,A8,30X,5HERROR/1H ,9X,11H-------PHA5800
     1----,20X,8H--------,22X,21H----------------------/1H ,7X,4HT(2),8X,PHA5810
     24HT(1),9X,8HOBSERVED,8X,10HCALCULATED,6X,10HDIFFERENCE,4X,7HPERCENPHA5820
     3T,2X,14HOBS-CALC/SIGYO)                                            PHA5830
 7300 FORMAT (1H ,2F12.3,1P2D17.4,0P3F13.4)                              PHA5840
 7400 FORMAT (55H0THE ARITHMETIC MEAN  OF THE ERRORS FOR THIS SET ARE --PHA5850
     1--- ,3F13.4/59H0THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -------PHA5860
     2------- ,3F13.4/31H0THE NUMBER OF OBSERVATIONS IS ,I5)             PHA5870
 7500 FORMAT (1H0,10A8/1H )                                              PHA5880
 7600 FORMAT (1H0,T35,21HTEMPERATURE (KELVINS))                          PHA5890
 7700 FORMAT (1H0/1H ,A8/1H0)                                            PHA5900
 7800 FORMAT (1H ,15X,A8,8X,A8,8X,A8,8X,A8,8X,A8,8X,A8,8X,A8/1H )        PHA5910
 7900 FORMAT (1H0,F7.2,2F16.3,2F16.0,2F16.4,F16.0)                       PHA5920
 8000 FORMAT (1H0,10X,3H'A',15X,3H'B',15X,3H'C',15X,3H'D',15X,3H'E',15X,PHA5930
     13H'F',15X,3H'G'/1H0,1P7D18.7)                                      PHA5940
 8100 FORMAT (35H I,YOUR FRIENDLY COMPUTER, DO NOW QUIT./9H0IN YOUR ,I4,PHA5950
     146TH DATA SET YOU HAVE MISSTYPED THE PHASE NAME.)                  PHA5960
 8200 FORMAT (1P6D12.5,A8)                                               PHA5970
 8300 FORMAT (1P1D12.5,52X,2A8)                                          PHA5980
 8400 FORMAT (7A8,8X,2A8)                                                PHA5990
 8500 FORMAT (7A8,8HCOMPLETE,2A8)                                        PHA6000
      END                                                                PHA6010-
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      BLOCK DATA                                                          BLK  10
      IMPLICIT REAL*8(A-H,O-Z)                                            BLK  20
      LOGICAL*1 BCD,LABEL                                                 BLK  30
      DIMENSION SCINV(2),STCOEF(10I,YESNO(2),TK(19,2I,TYPE(14),NSCALE(5IBLK  40
     1  ,LABEL(50)                                                        BLK  50
C     ------------------------------------------------------------------BLK  60
C         COMMON BLOCKS                                                 BLK  70
C            NAME              ROUTINES                                 BLK  80
C              EARTH             MAIN PROGRAM, ORBLS2, EAFW2D, PUTOUT   BLK  90
C              AIR               MAIN PROGRAM, ORBLS2, TEST2D, EAFW2D   BLK 100
C                                PUTOUT AND UNICLE.                     BLK 110
C              FIRE              MAIN PROGRAM, ORBLS2, TEST2D, EAFW2D   BLK 120
C              WATER             MAIN PROGRAM, EAFW2D, YDERIV, DDERIV,  BLK 130
C                                PUTOUT, EN, DIF, AND BLOCK DATA.       BLK 140
C              TIME              MAIN PROGRAM, PLTOUT                   BLK 150
C              SPACE             MAIN PROGRAM, EAFW2D, YDERIV, DDERIV,  BLK 160
C                                   AND PUTPLT                          BLK 170
C              MAN               MAIN PROGRAM, PLTPLT                   BLK 180
C     ------------------------------------------------------------------BLK 190
      COMMON /JOULES/UNITS                                                BLK 200
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,               BLK 210
     1  SCINV, TREF, STCOEF, DIEO, A, B, THETA, YESNO, TK,                BLK 220
     2  ASTAR, TYPE, NL, NSCALE, LABEL, BCD                               BLK 230
C     ------------------------------------------------------------------BLK 240
C     THE FOLLOWING VALUES OF 'R' AND 'F' ARE TO BE USED FOR ENERGY       BLK 250
C        DATA IN CALORIES.                                                BLK 260
C     DATA R,F/4.575616500,2.306094604/                                   BLK 270
C     THE FOLLOWING VALUES OF 'R' AND 'F' ARE TO BE USED FOR ENERGY       BLK 280
C        DATA IN JOULES.                                                  BLK 290
C     DATA R,F/19.144379D0,9.648700D4/                                    BLK 300
C     ------------------------------------------------------------------BLK 310
      DATA UNITS/8H JOULES /                                              BLK 320
      DATA R,F/19.144379DC,9.648700D4/                                    BLK 330
      DATA ZERO,ONE,TWO,THREE,FOUR,SIX/0.0D0,1.0DC,2.0DC,3.000,4.0D0,     BLK 340
     I  6.CDO/                                                            BLK 350
      DATA SCINV/-1.0D0,1.CC0/                                            BLK 360
      DATA TREF/2.9815D2/                                                 BLK 370
      DATA  STCOEF /1.0C0,2.0D0,3.000,4.0C0,5.0C0,0.5D0,0.400,0.33333333BLK 380
     133D0,0.25C0,C.200/                                                  BLK 390
      DATA DIEC,A,B,THETA/3.057D2,1.875C-2,-1.2741D1,2.1902/              BLK 400
      DATA YESNC     /3HNO ,3HYES/                                        BLK 410
      DATA TYPE      /8HHEAT CAP,8HENTROPY ,8HENTHALPY,8HGIBBS EN,        BLK 420
     1     8HLOG K   ,8HCELL EMF,8HHT2-HT1 ,7*8HSPECIAL /                BLK 430
      DATA ASTAR/8H********/                                              BLK 440
      DATA TK /273.15D0,298.15D0,323.15D0,348.15D0,373.15D0,398.15D0,     BLK 450
     1 423.15D0,448.15D0,473.15D0,498.15D0,523.15D0,548.15D0,573.15D0,    BLK 460
     2 598.15D0,623.15DC,C.CD0,0.0D0,0.0D0,0.0DC,273.15DC,298.15D0,      BLK 470
     3 4.0D2,5.0D2,6.0D2,7.0D2,8.0D2,9.0D2,1.0D3,1.1D3,1.2D3,1.3D3,      BLK 480
     4 1.4D3,1.5D3,1.6D3,1.7D3,1.8D3,1.9D3,2.0D3/                        BLK 490
      DATA LABEL /30HOBS LESS CALC OVER UNCERTAINTY/                      BLK 500
      DATA NL/3C/                                                         BLK 510
      DATA BCD/1HO/                                                       BLK 520
      DATA NSCALE/5*0/                                                    BLK 530
      END                                                                 BLK 540-
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      SUBROUTINE ORGLS2 (CALC)                                          CRG  10
C     ------------------------------------------------------------------ORG  20
C                                                                       CRG  30
C                                DR GLS                                 CRG  40
C                                                                       CRG  50
C           A GENERAL FORTRAN LEAST SQUARES PROGRAM                     CRG  60
C                                 BY                                    CRG  70
C              WILLIAM R. BUSING AND HENRI A. LEVY                      CRG  80
C                       CHEMISTRY DIVISION                              CRG  90
C                  OAK RIDGE NATIONAL LABORATORY                        CRG 100
C                      OAK RIDGE, TENNESSEE                             CRG 110
C                                                                       CRG 120
C     REFERENCE-- BUSING, W. R. AND LEVY, H. A., 1962, OR GLS, A GENERALCRG 130
C                   FORTRAN LEAST SQUARES PROGRAM, OAK RIDGE            CRG 140
C                   NATIONAL LABORATORY, OAK RIDGE, TENN.,              CRG 150
C                   ORNL-TM-271.                                        CRG 160
C                                                                       CRG 170
C                                                                       CRG 180
C                              SUBROUTINE CRGLS2                        CRG 190
C                                                                       CRG 200
C          ORGLS2 HAS BEEN ADAPTED FROM BUSING AND LEVY'S OR GLS        CRG 210
C     PROGRAM TO ALLOW USE OF THE STATISTICAL ROUTINES WITHOUT BEING    CRG 220
C     RESTRICTED TO THE RIGID INPUT-OUTPUT FEATURES OF THE PROGRAM.     CRG 230
C     THE CONVERSION HAS PERMITTED CHANGES WHICH CLARIFY THE OUTPUT     CRG 240
C     FOR THIS PECULIAR PROBLEM.                                        CRG 250
C                                                                       CRG 260
C     ADAPTATION BY HAAS, 8/20/72.                                      CRG 270
C                                                                       CRG 280
C                                                                       CRG 290
C     ------------------------------------------------------------------CRG 300
       IMPLICIT REAL*8 (A-H,O-Z)                                        CRG 310
      REAL*4 TITLE,PCTERR,CUT                                           CRG 320
      DIMENSION OUT(7)                                                  CRG 330
      DIMENSION SQSIG(2),AM(10010),V(140),CV(140),DIAG(140),RCW(140)    CRG 340
      DIMENSION CCEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),         CRG 350
     1  NPHASE(70),IKOUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),        CRG 360
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                          CRG 370
      DIMENSION X(2,1200),YC(1200),SIGYC(1200),P(140),KI(140),          CRG 380
     1  CG(140),PD(140),TITLE(20)                                       CRG 390
      DIMENSION REF(10,70),ERRP(140),IHOLD(40)                          CRG 400
C     ------------------------------------------------------------------CRG 410
C         COMMON BLOCKS                                                 CRG 420
C            NAME              ROUTINES                                 CRG 430
C              EARTH             MAIN PROGRAM, ORGLS2, EAFW20, PUTOUT   CRG 440
C              AIR               MAIN PROGRAM, ORGLS2, TEST20, EAFW20   CRG 450
C                                PUTOUT AND UNIQUE.                     CRG 460
C              FIRE              MAIN PROGRAM, ORGLS2, TEST20, EAFW20   CRG 470
C              WATER             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  CRG 480
C                                PUTOUT, FN, DIE, AND PLOCK DATA.       CRG 490
C              TIME              MAIN PROGRAM, PUTOUT                   CRG 500
C              SPACE             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  CRG 510
C                                   AND PUTPUT                          CRG 520
C              MAN               MAIN PROGRAM, PUTOUT                   CRG 530
C     ------------------------------------------------------------------CRG 540
      COMMON /EARTH/ CCEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGO,NSETS,    CRG 550
     I  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                          CRG 560
      COMMON /AIR/ X, P, DC, TITLE, YO, SIGYD, PD, KI, NC, NV, NX, IW,  CRG 570
     1  NP, NO, ISING, ISTOP, IL, JOFLAG                                CRG 580
      COMMON /FIRE/ REF, ERRP, IWRITE, ICY, IICY, IREDC, IREG, NHOLD,   CRG 590
     1 IHOLD                                                            CRG 600
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C      FORMAT STATEMENTS                                                ORG 610
  100 FORMAT (1H1120A4)                                                 ORG 620
  200 FORMAT (32HONUMBER OF CYCLES IN THIS JOB ISI2/37HONUMBER OF PARAMSORG 630
     1TERS TO BE VARIED ISI3/51HONUMBER OF INDEPENDENT VARIABLES PER OBSORG 640
     2ERVATION ISI2)                                                    ORG 650
  300 FORMAT (46HODERIVATIVES PROGRAMMED IN SUBROUTINE EAFW20. )        ORG 660
  400 FORMAT (31HOWEIGHTS TO BE SUPPLIED BY USER)                       ORG 670
  500 FORMAT (34HOUNIT WEIGHTS TO BE SET BY PROGRAM)                    ORG 680
  600 FORMAT (25HONUMBER OF PARAMETERS READ ISI4)                       ORG 690
  700 FORMAT (31HONUMBER OF OBSERVATIONS READ ISI5)                     ORG 700
  800 FORMAT (46HOCALCULATED Y BASED ON PARAMETERS BEFORE CYCLEI2)      ORG 710
  900 FORMAT (1H0,10X,5HINDEX,7X,4HT(2),8X,4HT(1),10X,6HY(OBS),10X,7HY(CORG 720
     1ALC),8X,8HOBS-CALC,9X,6HSIG(O),6X,12H(O-C)/SIG(C))                ORG 730
 1000 FORMAT (1H ,I15,F12.3,12X,1P4D16.3,0PF16.4)                       ORG 740
 1100 FORMAT (1H ,I15,2F12.3,1P4D16.3,0PF16.4)                          ORG 750
 1200 FORMAT (1H ,I15,F12.3,12X,5F16.4)                                 ORG 760
 1300 FORMAT (1H ,I15,2F12.3,5F16.4)                                    ORG 770
 1400 FORMAT (51HOAGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLEI2/2ORG 780
     1OHOSUM(W*(O-C)**2) IS D11.3/35HOSQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS ORG 790
     2D10.4)                                                            ORG 800
 1500 FORMAT (6CHOESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER ORG 810
     1CYCLEI2/2OHOSUM(W*(O-C)**2) IS D11.3/35HOSQRTF(SUM(W*(O-C)**2)/(NOORG 820
     2-NV)) IS D10.4)                                                   ORG 830
 1600 FORMAT (62H MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PAORG 840
     1RAMETERI3,16H OF THOSE VARIED)                                    ORG 850
 1700 FORMAT (40H SINGULARITY RETURN FROM MATRIX INVERTER)              ORG 860
 1800 FORMAT (37HOPARAMETERS AFTER LEAST SQUARES CYCLEI2/1HO,T16,'OLD',TORG 870
     135,'CHANGE',T57,'NEW',T77,'ERROR',T95,'PCT. CHANGE',T118,'PCT. ERRORG 880
     2OR'/1H )                                                          ORG 890
 1900 FORMAT (1H0,A8)                                                   ORG 900
 2000 FORMAT (1H I3,2(4X,1PD17.10))                                     ORG 910
 2100 FORMAT (1H ,I3,1P5D21.10,0PF17.4)                                 ORG 920
 2200 FORMAT (66HOSUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATEDORG 930
     1 FOR REASONI2)                                                    ORG 940
 2300 FORMAT (16HOTRIAL CONSTANTS/1HO,2X,1HI,9X,4HP(I),6X,5HKI(I)/1H ) ORG 950
 2400 FORMAT (1H0,9X,A8)                                                ORG 960
 2500 FORMAT (1H ,I3,5X,1PD11.4,6X,I1)                                  ORG 970
 2600 FORMAT (19HOCORRELATION MATRIX)                                   ORG 980
 2700 FORMAT (1H0I3,10D12.4/(1H 3X,10D12.4))                            ORG 990
 2800 FORMAT (14H1***WARNING***/93HOTHE TERM SIG/(NO-NV) IS NEGATIVE.  TORG1000
     1HE ABSOLUTE VALUE IS TAKEN AND THE REGRESSION CONTINUES.)         ORG1010
      DO 2900 I=1,NP                                                    ORG1020
      ERRP(I)=0.0D0                                                     ORG1030
 2900 CONTINUE                                                          ORG1040
      WRITE (6,100) (TITLE(I),I=1,20)                                   ORG1050
      WRITE (6,200) NO,NV,NX                                            ORG1060
      WRITE (6,300)                                                     ORG1070
      IF (IW) 3100,3000,3100                                            ORG1080
 3000 WRITE (6,400)                                                     ORG1090
      GO TO 3200                                                        ORG1100
 3100 WRITE (6,500)                                                     ORG1110
 3200 CONTINUE                                                          ORG1120
      WRITE (6,600) NP                                                  ORG1130
      WRITE (6,700) NO                                                  ORG1140
      IF (NO) 3300,3300,3500                                            ORG1150
 3300 DO 3400 I=1,NP                                                    ORG1160
 3400 KI(I)=0                                                           ORG1170
C     INITIALIZE PROBLEM AND ENTER SUBROUTINE PRELIM IF PROVIDED        ORG1180
 3500 NM=(NV*(NV+1))/2                                                  ORG1190
      SQSIG(1)=0.0D0                                                    ORG1200
      CALL PRELIM                                                       ORG1210
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C     PUT OUT TRIAL PARAMETERS, AND KEY-INTEGERS.                        ORG1220
      WRITE (6,2300)                                                     ORG1230
      JO=1                                                               ORG1240
      DO 3600 I=1,LISTP                                                  ORG1250
      WRITE (6,2400) PNAME(I)                                            ORG1260
      JN=JO+6                                                            ORG1270
      WRITE (6,2500) (J,P(J),KI(J),J=JO,JN)                              ORG1280
      JO=JO+7                                                            ORG1290
 3600 CONTINUE                                                           ORG1300
C     START LOOP TO PERFORM NC CYCLES AND ONE FINAL CALCULATION OF Y     ORG1310
      NCY=NC+1                                                           ORG1320
      DO 7900 IC=1,NCY                                                   ORG1330
C        CLEAR ARRAYS AM AND V EXCEPT ON LAST CYCLE                      ORG1340
      IF (IC-NCY) 3700,4000,4000                                         ORG1350
 3700 DO 3800 I=1,NM                                                     ORG1360
 3800 AM(I)=0.000                                                        ORG1370
      DO 3900 I=1,NV                                                     ORG1380
 3900 V(I)=0.000                                                         ORG1390
C        INITIALIZE FOR CYCLE IC AND PUT OUT CAPTION FOR LIST OF Y(CALC) ORG1400
 4000 SQSIG(2)=SQSIG(1)                                                  ORG1410
      SIG=0.000                                                          ORG1420
      WRITE (6,100) (TITLE(I),I=1,20)                                    ORG1430
      IF (IL.NE.0) GO TO 4100                                            ORG1440
      IF (IC.NE.NCY) GO TO 4200                                          ORG1450
 4100 CONTINUE                                                           ORG1460
      WRITE (6,800) IC                                                   ORG1470
      WRITE (6,900)                                                      ORG1480
 4200 CONTINUE                                                           ORG1490
C        START LOOP THROUGH NO OBSERVATIONS                              ORG1500
      DO 5900 I=1,NO                                                     ORG1510
C           ENTER USERS SUBROUTINE TO COMPUTE Y(CALC) AND DERIVATIVES    ORG1520
      CALL CALC (YC,I)                                                   ORG1530
C           OBTAIN WEIGHT AND CALCULATE QUANTITIES FROM Y(OBS)-Y(CALC)   ORG1540
      IF (IW) 4400,4300,4400                                             ORG1550
 4300 SQRTW=1.000/SIGYC(I)                                               ORG1560
      GO TO 4500                                                         ORG1570
 4400 SIGYO(I)=1.000                                                     ORG1580
      SQRTW=1.000                                                        ORG1590
 4500 DY=YO(I)-YC                                                        ORG1600
      WDY=SQRTW*DY                                                       ORG1610
      SIG=SIG+WDY*WDY                                                    ORG1620
C           PUT OUT Y(CALC) AND OTHER INFORMATION FOR ONE OBSERVATION    ORG1630
      IF (IL.NE.0) GO TO 4600                                            ORG1640
      IF (IC.NE.NCY) GO TO 5100                                          ORG1650
 4600 CONTINUE                                                           ORG1660
      OUT(1)=X(1,I)                                                      ORG1670
      OUT(2)=X(2,I)                                                      ORG1680
      OUT(3)=YO(I)                                                       ORG1690
      OUT(4)=YC                                                          ORG1700
      OUT(5)=DY                                                          ORG1710
      OUT(6)=SIGYO(I)                                                    ORG1720
      OUT(7)=WDY                                                         ORG1730
      IF (X(2,I).EQ.0.000) GO TO 4800                                    ORG1740
      IF ((DABS(YO(I)).LT.1.0D-3).AND.(YO(I).NE.0.000)) GO TO 4700       ORG1750
      WRITE (6,1300) I,(OUT(K),K=1,7)                                    ORG1760
      GO TO 5000                                                         ORG1770
 4700 CONTINUE                                                           ORG1780
      WRITE (6,1100) I,OUT(1),OUT(2),YO(I),YC,DY,SIGYC(I),OUT(7)         ORG1790
      GO TO 5000                                                         ORG1800
 4800 CONTINUE                                                           ORG1810
      IF ((DABS(YO(I)).LT.1.0D-3).AND.(YO(I).NE.0.000)) GO TO 4900       ORG1820
```

```
      WRITE (6,4200) I,CUT(1),(OUT(K),K=3,7)                            ORG1830
      GO TO 5000                                                        ORG1840
 4900 CONTINUE                                                          ORG1850
      WRITE (6,1000) I,CUT(1),YO(I),YC,DY,SIGYC(I),OUT(7)               ORG1860
 5000 CONTINUE                                                          ORG1870
 5100 CONTINUE                                                          ORG1880
C           BY-PASS DERIVATIVE AND MATRIX SET-UP ON FINAL CALC OF Y     ORG1890
      IF (IC-NCY) 5200,5900,5900                                        ORG1900
C             START LOOP TO STORE AN ARRAY OF NV DERIVATIVES            ORG1910
 5200 J=1                                                               ORG1920
      DO 5400 K=1,NP                                                    ORG1930
      IF (KI(K)) 5400,5400,5300                                         ORG1940
 5300 CONTINUE                                                          ORG1950
C                       OBTAIN DERIVATIVE FROM THOSE PROGRAMMED BY USER ORG1960
      DV(J)=SQRTW*DC(K)                                                 ORG1970
      J=J+1                                                             ORG1980
 5400 CONTINUE                                                          ORG1990
C                 END LOOP TO OBTAIN DERIVATIVES                       ORG2000
C             START LOOP TO STORE MATRIX AND VECTOR.                   ORG2010
C             1604 OR CLS STORAGE SCHEME IS REVERSE OF 7090 OR GLS     ORG2020
      JK=1                                                              ORG2030
      DO 5800 J=1,NV                                                    ORG2040
      TEMP=DV(J)                                                        ORG2050
      IF (TEMP) 5600,5500,5600                                          ORG2060
C                     BY-PASS IF DERIVATIVE IS ZERO                     ORG2070
 5500 JK=JK+NV+1-J                                                      ORG2080
      GO TO 5800                                                        ORG2090
 5600 DO 5700 K=J,NV                                                    ORG2100
      AM(JK)=AM(JK)+TEMP*DV(K)                                          ORG2110
      JK=JK+1                                                           ORG2120
 5700 CONTINUE                                                          ORG2130
      V(J)=V(J)+TEMP*WDY                                                ORG2140
 5800 CONTINUE                                                          ORG2150
C                     END LOOP TO STORE MATRIX AND VECTOR               ORG2160
 5900 CONTINUE                                                          ORG2170
C               END LOOP THROUGH NO OBSERVATIONS                        ORG2180
C        COMPUTE AND PUT OUT AGREEMENT FACTORS                          ORG2190
      CNVN=NO-NV                                                        ORG2200
      SQSIG(1)=DSQRT(SIG/(CNVN))                                        ORG2210
      WRITE (6,1400) IC,SIC,SQSIG(1)                                    ORG2220
C        BY-PASS MATRIX INVERSION AND PARAMETER OUTPUT ON FINAL CYCLE   ORG2230
      IF (IC-NCY) 6000,8000,8000                                        ORG2240
C             START LOOP TO TEST FOR ZERO DIAGONAL ELEMENT              ORG2250
 6000 ISING=0                                                           ORG2260
      II=1                                                              ORG2270
      IID=NV                                                            ORG2280
      DO 6300 I=1,NV                                                    ORG2290
      IF (AM(II)) 6200,6100,6200                                        ORG2300
 6100 ISING=1                                                           ORG2310
      WRITE (6,1600) I                                                  ORG2320
 6200 II=II+IID                                                         ORG2330
      IID=IID-1                                                         ORG2340
 6300 CONTINUE                                                          ORG2350
C               END LOOP TO TEST FOR ZERO DIAGONAL ELEMENT              ORG2360
C            TERMINATE JOB IF ZERO DIAGONAL ELEMENT WAS FOUND           ORG2370
      IF (ISING) 8600,6400,8600                                         ORG2380
C               ENTER SUBROUTINE TO REPLACE MATRIX WITH INVERSE         ORG2390
 6400 CALL MINV2G (AM,NV,ISING)                                         ORG2400
      IF (ISING) 6500,6600,6500                                         ORG2410
C                  TERMINATE JOB IF SINGULAR MATRIX WAS FOUND          ORG2420
 6500 WRITE (6,1700)                                                    ORG2430
```

```
      GO TO 8600                                                        ORG2440
C                  START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR      ORG2450
C                                                  PARAMETER CHANGES    ORG2460
 6600 DO 7100 I=1,NV                                                    ORG2470
      PDI=0.000                                                         ORG2480
      IJ=I                                                              ORG2490
      IJD=NV-1                                                          ORG2500
      DO 7000 J=1,NV                                                    ORG2510
      PDI=PDI+AM(IJ)*V(J)                                               ORG2520
      IF (J-I) 6700,6800,6900                                           ORG2530
 6700 IJ=IJ+IJD                                                         ORG2540
      IJD=IJD-1                                                         ORG2550
      GO TO 7000                                                        ORG2560
C                          SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX     ORG2570
 6800 DIAG(I)=AM(IJ)                                                    ORG2580
 6900 IJ=IJ+1                                                           ORG2590
 7000 CONTINUE                                                          ORG2600
      PD(I)=PDI                                                         ORG2610
      SIG=SIG-PDI*V(I)                                                  ORG2620
 7100 CONTINUE                                                          ORG2630
C                    END LOOP FOR MATRIX VECTOR MULTIPLICATION         ORG2640
C                  RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG       ORG2650
      IF (SIG) 7200,7300,7300                                           ORG2660
 7200 CONTINUE                                                          ORG2670
      WRITE (6,2800)                                                    ORG2680
      SIG=DABS(SIG)                                                     ORG2690
 7300 CONTINUE                                                          ORG2700
      SQSIG(1)=DSQRT(SIG/(NC-NV))                                       ORG2710
C                  PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS    ORG2720
      WRITE (6,100) (TITLE(I),I=1,20)                                   ORG2730
      WRITE (6,1800) IC                                                 ORG2740
C                  START LOOP TO CORRECT AND PUT OUT PARAMETERS        ORG2750
      J=1                                                               ORG2760
      JO=1                                                              ORG2770
      DO 7700 IC=1,LISTP                                                ORG2780
      WRITE (6,1900) PNAME(IO)                                          ORG2790
      JN=JO+6                                                           ORG2800
      DO 7600 I=JO,JN                                                   ORG2810
      IF (KI(I)) 7400,7400,7500                                         ORG2820
 7400 WRITE (6,2000) I,P(I),P(I)                                        ORG2830
      GO TO 7600                                                        ORG2840
 7500 POLD=P(I)                                                         ORG2850
      P(I)=POLD+PD(J)                                                   ORG2860
      SIGP=DSQRT(DIAG(J))*SQSIG(1)                                      ORG2870
      PCTCHG=1.02*PD(J)/P(I)                                            ORG2880
      PCTERR=DABS(1.002*SIGP/P(I))                                      ORG2890
      ERRP(I)=PCTERR                                                    ORG2900
      WRITE (6,2100) I,POLD,PD(J),P(I),SIGP,PCTCHG,PCTERR               ORG2910
      J=J+1                                                             ORG2920
 7600 CONTINUE                                                          ORG2930
      JO=JO+7                                                           ORG2940
 7700 CONTINUE                                                          ORG2950
C                    END LOOP TO CORRECT AND PUT OUT PARAMETERS         ORG2960
C                  PUT OUT ESTIMATED AGREEMENT FACTORS                 ORG2970
      WRITE (6,1500) IC,SIG,SQSIG(1)                                    ORG2980
C                  ENTER USERS SUBROUTINE TO TEST AND MODIFY PARAMETERS ORG2990
C                                                      OR END JOB      ORG3000
      ISTOP=0                                                           ORG3010
      CALL TEST20                                                       ORG3020
C                  TERMINATE JOB IF INDICATED BY USERS SUBROUTINE TEST ORG3030
      IF (ISTOP) 7800,7900,7800                                         ORG3040
```

```
 7800 WRITE (6,2200) ISTOP                                              ORG3050
      GO TO 8000                                                        CRG3060
 7900 CONTINUE                                                          CRG3070
C                    END LOOP THROUGH NC CYCLES AND FINAL CALC OF Y     CRG3080
C     TERMINATE JOB                                                    CRG3090
 8000 IF (NC) 8600,8600,8100                                            ORG3100
C        CALCULATE AND PUT OUT CORRELATION MATRIX                      CRG3110
 8100 WRITE (6,1000) (TITLE(I),I=1,20)                                  CRG3120
      WRITE (6,2600)                                                    ORG3130
      DO 8200 I=1,NV                                                    ORG3140
      DIAG(I)=1.000/DSQRT(DIAG(I))                                      ORG3150
 8200 CONTINUE                                                          ORG3160
      IJ=1                                                              ORG3170
      DO 8500 I=1,NV                                                    ORG3180
      DO 8300 J=1,NV                                                    ORG3190
      ROW(J)=0.000                                                      ORG3200
 8300 CONTINUE                                                          ORG3210
      DO 8400 J=I,NV                                                    ORG3220
      ROW(J)=AM(IJ)*DIAG(I)*DIAG(J)                                     ORG3230
      IJ=IJ+1                                                           ORG3240
 8400 CONTINUE                                                          ORG3250
      WRITE (6,2700) I,(ROW(J),J=1,NV)                                  ORG3260
 8500 CONTINUE                                                          CRG3270
 8600 CONTINUE                                                          CRG3280
      RETURN                                                            ORG3290
      END                                                               ORG3300-
```

```
      SUBROUTINE PRELIM                                                 PRE 001
C     - - ----------------------------------------------------------- PRE 002
C          DUMMY SUBROUTINE PRELIM                                      PRE 003
C     ----------- ----------------------------------------------------- PRE 004
      RETURN                                                            PRE 005
      END                                                               PRE 006
```

```
      SUBROUTINE TEST20                                                 TES  10
C     ------------------------------------------------------------------TES  20
C                                                                       TES  30
C                                     TEST20                            TES  40
C                                                                       TES  50
C     TEST20 TERMINATES THE REGRESSION IF THE CHANGE IN ALL             TES  60
C          PARAMETERS IS LESS THAN 1.0D-8.                              TES  70
C                                                                       TES  80
C     TEST20  WILL ALSO CAUSE IREDO TO TAKE THE INDEX OF THE            TES  90
C          PARAMETER WHICH HAS THE GREATEST ERROR, PROVIDED ICY HAS     TES 100
C          AN NON-ZERO VALUE AND PROVIDED THE ERROR ON ONE OR MORE      TES 110
C          PARAMETERS IS GREATER THAN 10 PERCENT.                       TES 120
C                                                                       TES 130
C     ------------------------------------------------------------------TES 140
       IMPLICIT REAL*8 (A-H,O-Z)                                        TES 150
       REAL*4 TITLE                                                     TES 160
       DIMENSION X(2,1200),YO(1200),SIGYO(1200),P(140),KI(140),         TES 170
      1  DO(140),PO(140),TITLE(20)                                      TES 180
       DIMENSION REF(10,70),ERRP(140),IHOLD(40)                         TES 190
C     ------------------------------------------------------------------TES 200
C                                                                       TES 210
C         COMMON BLOCKS                                                 TES 220
C            NAME              ROUTINES                                 TES 230
C              EARTH             MAIN PROGRAM, ORGLS2, EAFW20, PUTOUT   TES 240
C              AIR               MAIN PROGRAM, ORGLS2, TEST20, EAFW20   TES 250
C                                PUTOUT AND UNIGLE.                     TES 260
C              FIRE              MAIN PROGRAM, ORGLS2, TEST20, EAFW20   TES 270
C              WATER             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  TES 280
C                                PUTOUT, FN, DIF, AND BLOCK DATA.       TES 290
C              TIME              MAIN PROGRAM, PLTOUT                   TES 300
C              SPACE             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  TES 310
C                                   AND PUTPUT                          TES 320.
C              MAN               MAIN PROGRAM, PLTOUT                   TES 330
C     ------------------------------------------------------------------TES 340
       COMMON /AIR/ X, P, DO, TITLE, YO, SIGYO, FO, KI, NO, NV, NX, IW, TES 350
      1  NP, ND, ISING, ISTOP, IL, JOFLAG                               TES 360
       COMMON /FIRE/ REF, ERRP, IWRITE, ICY, IICY, IPEDO, IREG, NHOLO,  TES 370
      1 IHOLO                                                           TES 380
       IREDO=0                                                          TES 390
       ISTAY=0                                                          TES 400
       J=1                                                              TES 410
       DO 400 I=1,NP                                                    TES 420
       IF (KI(I).EQ.0) GO TO 400                                        TES 430
       IF (DABS(PO(J)/P(I)).GT.1.0D-8) ISTAY=1                          TES 440
       J=J+1                                                            TES 450
       IF (ICY.EQ.0) GO TO 400                                          TES 460
       DERRP=ERRP(I)                                                    TES 470
       IF (DERRP.LE.1.0D1) GO TO 400                                    TES 480
       IF (IREDO.EQ.0) GO TO 100                                        TES 490
       IF (DERRP.LE.ERRP(IREDO)) GO TO 400                              TES 500
   100 CONTINUE                                                         TES 510
       IF (NHOLD.EQ.0) GO TO 300                                        TES 520
       DO 200 K=1,NHOLO                                                 TES 530
       IF (I.EQ.IHOLD(K)) GO TO 400                                     TES 540
   200 CONTINUE                                                         TES 550
   300 CONTINUE                                                         TES 560
       IREDO=I                                                          TES 570
   400 CONTINUE                                                         TES 580
       IF (ISTAY.EQ.1) GO TO 500                                        TES 590
       ISTOP=1                                                          TES 600
   500 RETURN
```

END

TES 610-

```
      SUBROUTINE MINV20 (AM,N,NFAIL)                                    MIN  10
      IMPLICIT REAL*8(A-H,O-Z)                                          MIN  20
      DIMENSION AM(10010)                                               MIN  30
C     ********** SEGMENT 1 OF CHOLESKI INVERSION **********            MIN  40
C     ***** FACTOR MATRIX INTO LOWER TRIANGLE X TRANSPOSE *****         MIN  50
      K=1                                                               MIN  60
      IF (N-1) 100,200,300                                              MIN  70
  100 NFAIL=K                                                           MIN  80
      GO TO 2000                                                        MIN  90
  200 AM(1)=1.0/AM(1)                                                   MIN 100
      GO TO 1900                                                        MIN 110
C     ***** LOOP M OF A(L,M) *****                                      MIN 120
  300 DO 1200 M=1,N                                                     MIN 130
      IMAX=M-1                                                          MIN 140
C     ***** LOOP L OF A(L,M) *****                                      MIN 150
      DO 1100 L=M,N                                                     MIN 160
      SUMA=0.0                                                          MIN 170
      KLI=L                                                             MIN 180
      KMI=M                                                             MIN 190
      IF (IMAX) 600,600,400                                             MIN 200
C     *****SUM OVER I=1,M-1 A(L,I)*A(M,I) *****                         MIN 210
  400 DO 500 I=1,IMAX                                                   MIN 220
      SUMA=SUMA+AM(KLI)*AM(KMI)                                         MIN 230
      J=N-I                                                             MIN 240
      KLI=KLI+J                                                         MIN 250
  500 KMI=KMI+J                                                         MIN 260
C     *****TERM=C(L,M)-SUM *****                                        MIN 270
  600 TERM=AM(K)-SUMA                                                   MIN 280
      IF (L-M) 700,700,1000                                             MIN 290
  700 IF (TERM) 900,900,800                                             MIN 300
C     ***** A(M,M)=SQRT(TERM) *****                                     MIN 310
  800 DENOM=DSQRT(TERM)                                                 MIN 320
      AM(K)=DENOM                                                       MIN 330
      GO TO 1100                                                        MIN 340
  900 NFAIL=K                                                           MIN 350
      GO TO 2000                                                        MIN 360
C     ***** A(L,M)=TERM/A(M,M) *****                                    MIN 370
 1000 AM(K)=TERM/DENOM                                                  MIN 380
 1100 K=K+1                                                             MIN 390
 1200 CONTINUE                                                          MIN 400
C     ********** SEGMENT 2 OF CHOLESKI INVERSION **********            MIN 410
C     *****INVERSION OF TRIANGULAR MATRIX*****                          MIN 420
      AM(1)=1.0/AM(1)                                                   MIN 430
      KOM=1                                                             MIN 440
C     ***** STEP L OF B(L,M) *****                                      MIN 450
      DO 1500 L=2,N                                                     MIN 460
      KOM=KOM+N-L+2                                                     MIN 470
C     ***** RECIPROCAL OF DIAGONAL TERM *****                           MIN 480
      TERM=1.0/AM(KOM)                                                  MIN 490
      AM(KOM)=TERM                                                      MIN 500
      KMI=0                                                             MIN 510
      KLI=L                                                             MIN 520
      IMAX=L-1                                                          MIN 530
C     ***** STEP M OF B(L,M) *****                                      MIN 540
      DO 1400 M=1,IMAX                                                  MIN 550
      K=KLI                                                             MIN 560
C     ***** SUM TERMS *****                                             MIN 570
      SUMA=0.0                                                          MIN 580
      DO 1300 I=M,IMAX                                                  MIN 590
      II=KMI+I                                                          MIN 600
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      SUMA=SUMA-AM(KLI)*AM(III)                                          MIN 610
 1300 KLI=KLI+N-I                                                        MIN 620
C     ***** MULT SUM * RECIP OF DIAGONAL *****                          MIN 630
      AM(KI)=SUMA*TERM                                                   MIN 640
      J=N-M                                                              MIN 650
      KLI=K+J                                                            MIN 660
 1400 KMI=KMI+J                                                          MIN 670
 1500 CONTINUE                                                           MIN 680
C     ********** SEGMENT 3 OF CHOLESKI INVERSION **********             MIN 690
C     *****PREMULTIPLY LOWER TRIANGLE BY TRANSPOSE*****                  MIN 700
      K=1                                                                MIN 710
      DO 1800 M=1,N                                                      MIN 720
      KLI=K                                                              MIN 730
      DO 1700 L=M,N                                                      MIN 740
      KMI=K                                                              MIN 750
      IMAX=N-L+1                                                         MIN 760
      SUMA=0.0                                                           MIN 770
      DO 1600 I=1,IMAX                                                   MIN 780
      SUMA=SUMA+AM(KLI)*AM(KMI)                                          MIN 790
      KLI=KLI+1                                                          MIN 800
 1600 KMI=KMI+1                                                          MIN 810
      AM(K)=SUMA                                                         MIN 820
 1700 K=K+1                                                              MIN 830
 1800 CONTINUE                                                           MIN 840
 1900 NFAIL=0                                                            MIN 850
 2000 RETURN                                                             MIN 860
      END                                                                MIN 870-
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      SUBROUTINE EAFW20 (YC,I)                                          EAF  10
C     ------------------------------------------------------------------EAF  20
C                                                                       EAF  30
C                                  EAFW20                               EAF  40
C                                                                       EAF  50
C     THIS VERSION WRITTEN 3/09/72 BY HAAS.                             EAF  60
C         LAST MODIFIED 8/05/72 BY HAAS.                                EAF  70
C                                                                       EAF  80
C     ------------------------------------------------------------------EAF  90
      IMPLICIT REAL*8(A-H,O-Z)                                          EAF 100
      LOGICAL*1 BCC,LABEL                                               EAF 110
      REAL*4 TITLE                                                      EAF 120
      DIMENSION SGN(2)                                                  EAF 130
      DIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),         EAF 140
     1  NPHASE(70),IKOUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),        EAF 150
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                          EAF 160
      DIMENSION X(2,1200),YO(1200),SIGYO(1200),P(140),KI(140),          EAF 170
     1  CC(140),PD(140),TITLE(20)                                       EAF 180
      DIMENSION REF(10,70),ERRP(140),IHOLD(40)                          EAF 190
      DIMENSION SCINV(2),STCOEF(10),YESNO(2),TK(19,2),TYPE(14),NSCALE(5)EAF 200
     1  ,LABEL(50)                                                      EAF 210
      DIMENSION DDCC(7),DYCC(7)                                         EAF 220
C     ------------------------------------------------------------------EAF 230
C         COMMON BLOCKS                                                 EAF 240
C            NAME              ROUTINES                                 EAF 250
C              EARTH             MAIN PROGRAM, ORGLS2, EAFW20, PUTOUT   EAF 260
C              AIR               MAIN PROGRAM, ORGLS2, TEST20, EAFW20   EAF 270
C                                PUTOUT AND UNIQUE.                     EAF 280
C              FIRE              MAIN PROGRAM, ORGLS2, TEST20, EAFW20   EAF 290
C              WATER             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  EAF 300
C                                PUTOUT, FN, DIE, AND BLOCK DATA.       EAF 310
C              TIME              MAIN PROGRAM, PUTOUT                   EAF 320
C              SPACE             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  EAF 330
C                                   AND PUTPUT                          EAF 340
C              MAN               MAIN PROGRAM, PUTOUT                   EAF 350
C     ------------------------------------------------------------------EAF 360
      COMMON /EARTH/ COEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGO,NSETS,    EAF 370
     1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                          EAF 380
      COMMON /AIR/ X, P, DC, TITLE, YO, SIGYO, PD, KI, NC, NV, NX, IW,  EAF 390
     1  NP, ND, ISING, ISTOP, IL, JDFLAG                                EAF 400
      COMMON /FIRE/ REF, ERRP, IWRITE, ICY, IICY, IREDC, IREG, NHOLD,   EAF 410
     1 IHOLD                                                           EAF 420
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,             EAF 430
     1  SCINV, TREF, STCOEF, D1EO, ADIE, BDIE, THETA, YESNO, TK,        EAF 440
     2  ASTAR, TYPE, NL, NSCALE, LABEL, BCC                             EAF 450
      COMMON /SPACE/ DDCC, DYCC, SC, TO                                 EAF 460
      YC=ZERO                                                           EAF 470
      DO 100 K=1,NP                                                     EAF 480
      CC(K)=ZERO                                                        EAF 490
  100 CONTINUE                                                          EAF 500
C     ------------------------------------------------------------------EAF 510
C     DETERMINE J BY LOCATING I IN THE VECTOR IKOUNT.  IF NOT           EAF 520
C          LOCATED, PRINT ERROR MESSAGE AND STOP                        EAF 530
C     ------------------------------------------------------------------EAF 540
      DO 200 J=1,NSETS                                                  EAF 550
      IF (I.LE.IKOUNT(J)) GO TO 300                                     EAF 560
  200 CONTINUE                                                          EAF 570
      WRITE (6,2000)                                                    EAF 580
      STOP                                                              EAF 590
  300 CONTINUE                                                          EAF 600
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C     ------------------------------------------------------------------EAF 610
C     WRITE REFERENCE IF THE I-TH OBSERVATION IS THE FIRST IN THE       EAF 620
C          J-TH DATA SET.                                               EAF 630
C     ------------------------------------------------------------------EAF 640
      IF (IWRITE.EQ.1.OR.I.EQ.1) GO TO 400                              EAF 650
      GO TO 500                                                         EAF 660
  400 CONTINUE                                                          EAF 670
      WRITE (6,2100) (REF(II,JI,II=1,10I                               EAF 680
      IWRITE=0                                                          EAF 690
  500 CONTINUE                                                          EAF 700
      IF (I.EQ.IKOUNT(J)I IWRITE=)                                      EAF 710
      IF (IGO(JI.LE.7) GO TO 600                                        EAF 720
C     ------------------------------------------------------------------EAF 730
C     IF IGO(J) IS GREATER THAN 7, CALL UNIQUE TO CALCULATE             EAF 740
C        YC (AND THE DERIVATIVES DC(III IF JDFLAG (JN IN PHAS20) IS     EAF 750
C        ZERO).                                                         EAF 760
C     ------------------------------------------------------------------EAF 770
      CALL UNIQLE (YC,I,J,JDFLAG)                                       EAF 780
      RETURN                                                            EAF 790
  600 CONTINUE                                                          EAF 800
C     ------------------------------------------------------------------EAF 810
C     FOR EACH PHASE IN THE J-TH DATA SET, CALCULATE THE SEVEN          EAF 820
C          DERIVATIVES.                                                 EAF 830
C     ------------------------------------------------------------------EAF 840
      T=X(1,I)                                                          EAF 850
      TC=X(2,I)                                                         EAF 860
      LAST=NPHASE(J)                                                    EAF 870
      DO 1800 L=1,LAST                                                  EAF 880
C     ------------------------------------------------------------------EAF 890
C     LOCATE THE FIRST CONSTANT FOR THE L-TH PHASE IN THE VECTOR P.     EAF 900
C          INITIALIZE SC, THE STOICHIOMETRIC COEFFICIENT.               EAF 910
C     ------------------------------------------------------------------EAF 920
      INDEX=1+7*(IPHASE(L,J)-1)                                         EAF 930
      SC=COEF(L,J)                                                      EAF 940
C     ------------------------------------------------------------------EAF 950
C     CALL YDERIV TO CALCULATE THE TEMPERATURE TERM IN THE DERIVATIVE.  EAF 960
C          IF THE DATA SET IS FOR ENTROPY AND HEAT CAPACITY,  GO TO     EAF 970
C          STATEMENT 13C.                                               EAF 980
C     ------------------------------------------------------------------EAF 990
      IGOES=IGO(J)                                                      EAF1000
      IF (ISTATE(L,JI.EC.-1I IGOES=IGOES+7                              EAF1010
      CALL YDERIV (T,IGOESI    .                                        EAF1020
      IF (IGO(J).LE.2) GO TO 1600                                       EAF1030
C     ------------------------------------------------------------------EAF1040
C     CALL ODERIV TO CALCULATE THE DERIVATIVE WITH RESPECT TO -C- AT    EAF1050
C          298.15 KELVIN IF COMPONENT IS AN ELEMENT.  PROCEED TO ADJUST EAF1060
C          OC ACCORDINGLY.                                              EAF1070
C     ------------------------------------------------------------------EAF1080
      IF (ISTATE(L,J).NE.1) GO TO 600                                   EAF1090
      CALL ODERIV (TREFI                                                EAF1100
      DO 700 K=1,7                                                      EAF1110
      DC(K+INDEX-1I=DC(K+INDEX-1I+SC*ODOC(K)*OYCC(4)                    EAF1120
  700 CONTINUE                                                          EAF1130
      GO TO 1600                                                        EAF1140
  800 CONTINUE                                                          EAF1150
C     ------------------------------------------------------------------EAF1160
C     CHECK FOR INVERSIONS.  IF LOW TEMPERATURE PHASES ARE TO BE        EAF1170
C          CONSIDERED, INITIALIZE SGN.  IF LOW TEMPERATURE PHASES       EAF1180
C          ARE NOT TO BE CONSIDERED,  GO TO STATEMENT 100.              EAF1190
C     ------------------------------------------------------------------EAF1200
      IF (NINVER(L,J).LE.0I GO TO 1600                                  EAF1210
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```
      DO 900 LLL=1,2                                                    EAF1220
      SGN(LLL)=SCINV(LLL)                                               EAF1230
  900 CONTINUE                                                          EAF1240
      IF (INVSC(L,J).EQ.0) GO TO 1000                                   EAF1250
      SGN(1)=SGN(1)*STOCOEF(INVSC(L,J))                                 EAF1260
      SGN(2)=SGN(2)*STOCOEF(INVSC(L,J))                                 EAF1270
 1000 CONTINUE                                                          EAF1280
C     ------------------------------------------------------------------EAF1290
C     IF THE LOWEST TEMPERATURE PHASE IS AN ELEMENT, CALL DDERIV        EAF1300
C          THE ARGUMENT IS 298.15, AND PROCEED TO ADJUST DC             EAF1310
C          ACCORDINGLY.                                                 EAF1320
C     ------------------------------------------------------------------EAF1330
      IF (INSTAT(L,J).EQ.0) GO TO 1200                                  EAF1340
      IINVR=1+7*(INVPH(L,J,1)-1)                                        EAF1350
      CALL DDERIV (TREF)                                                EAF1360
      DO 1100 K=1,7                                                     EAF1370
      DC(K+IINVR-1)=DC(K+IINVR-1)+DDDC(K)*SGN(2)*SC*DYDC(4)             EAF1380
 1100 CONTINUE                                                          EAF1390
 1200 CONTINUE                                                          EAF1400
C     ------------------------------------------------------------------EAF1410
C     CALL DDERIV TO CALCULATE THE DERIVATIVE WITH RESPECT TO D FOR     EAF1420
C          HIGH AND LOW TEMPERATURE PHASE AT TEMPERATURE OF             EAF1430
C          INVERSION.  PROCEED TO ADJUST DC ACCORDINGLY.                EAF1440
C     ------------------------------------------------------------------EAF1450
      LSTINV=NINVER(L,J)                                                EAF1460
      DO 1500 LL=1,LSTINV                                               EAF1470
      CALL DDERIV (TINV(L,J,LL))                                        EAF1480
C     ------------------------------------------------------------------EAF1490
C                                                                       EAF1500
C                                                                       EAF1510
C     ------------------------------------------------------------------EAF1520
      IF (INVSC(L,J).EQ.0) GO TO 1300                                   EAF1530
      IF (LL.NE.LSTINV) GO TO 1300                                      EAF1540
      SGN(2)=SGN(2)/STOCOEF(INVSC(L,J))                                 EAF1550
 1300 CONTINUE                                                          EAF1560
      DO 1400 LLL=1,2                                                   EAF1570
      IINVR=1+7*(INVPH(L,J,(LL+LLL-1))-1)                               EAF1580
      DO 1400 K=1,7                                                     EAF1590
      DC(K+IINVR-1)=DC(K+IINVR-1)+DDDC(K)*SGN(LLL)*SC*DYDC(4)           EAF1600
 1400 CONTINUE                                                          EAF1610
 1500 CONTINUE                                                          EAF1620
 1600 CONTINUE                                                          EAF1630
C     ------------------------------------------------------------------EAF1640
C     COMPLETE THE CALCULATION OF DC BY ADDING THE DERIVATIVE AT T(OBS).EAF1650
C     ------------------------------------------------------------------EAF1660
      DO 1700 K=1,7                                                     EAF1670
      DC(K+INDEX-1)=DC(K+INDEX-1)+SC*DYDC(K)                            EAF1680
 1700 CONTINUE                                                          EAF1690
 1800 CONTINUE                                                          EAF1700
C     ------------------------------------------------------------------EAF1710
C     ALL DERIVATIVES HAVE BEEN CALCULATED.  NOW CALCULATE YC BY        EAF1720
C          SUMMING THE PRODUCT DC*P.                                    EAF1730
C     ------------------------------------------------------------------EAF1740
      DO 1900 K=1,NP                                                    EAF1750
      YC=YC+P(K)*DC(K)                                                  EAF1760
 1900 CONTINUE                                                          EAF1770
C     ------------------------------------------------------------------EAF1780
C     RETURN                                                            EAF1790
C     ------------------------------------------------------------------EAF1800
      RETURN                                                            EAF1810
C     ------------------------------------------------------------------EAF1820
```

```
C      FORMAT STATEMENTS                                                EAF1830
C      ------------------------------------------------------------------EAF1840
 2000 FORMAT (6CHOIN EAFm20 I IS GREATER THAN NC, THE NUMBER OF OBSERVATEAF1850
     1IONS./64H THEREFORE, I (THE COMPUTER) AM QUITTING. THE PROBLEM IS EAF1860
     2YOURS. )                                                         EAF1870
 2100 FORMAT (1H0,10A8/1H )                                            EAF1880
      END                                                              EAF1890-
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      SUBROUTINE YDERIV (T,J)                                           YDE  10
C     ------------------------------------------------------------------YDE  20
C                                                                       YDE  30
C                                   YDERIV                              YDE  40
C     THIS VERSION WRITTEN 3/09/72 BY HAAS.                             YDE  50
C          LAST REVISED 8/05/72 BY HAAS.                                YDE  60
C                                                                       YDE  70
C     ------------------------------------------------------------------YDE  80
      IMPLICIT REAL*8(A-H,O-Z)                                          YDE  90
      DIMENSION DYDC(7),SCINV(2),DDDC(7),STCOEF(10)                     YDE 100
C     ------------------------------------------------------------------YDE 110
C         COMMON BLOCKS                                                 YDE 120
C            NAME             ROUTINES                                 YDE 130
C              EARTH            MAIN PROGRAM, CRCLS2, EAFW20, PLTOLT   YDE 140
C              AIR              MAIN PROGRAM, CRCLS2, TEST20, EAFW20   YDE 150
C                               PUTOUT AND UNICLE.                     YDE 160
C              FIRE             MAIN PROGRAM, CRCLS2, TEST20, EAFW20   YDE 170
C              WATER            MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  YDE 180
C                               PUTOUT, FN, DIF, AND BLOCK DATA.       YDE 190
C              TIME             MAIN PROGRAM, PLTOUT                   YDE 200
C              SPACE            MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  YDE 210
C                                  AND PLTPLT                          YDE 220
C              FAN              MAIN PROGRAM, PLTOUT                   YDE 230
C     ------------------------------------------------------------------YDE 240
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,             YDE 250
     1  SCINV, TREF, STCOEF,DIDO,A,B,THETA                              YDE 260
      COMMON /SPACE/ DDDC, DYDC, SC, TC                                 YDE 270
C     ------------------------------------------------------------------YDE 280
C     CALCULATE THE APPROPRIATE TEMPERATURE TERM IN THE DERIVATIVE      YDE 290
C          AND RETURN.  --APPROPRIATE AS INDICATED BY J.                YDE 300
C     ------------------------------------------------------------------YDE 310
      GO TO (100,200,300,400,500,600,700,800,1000,1100,1200,1300,1400,15YDE 320
     1000), J                                                           YDE 330
  100 CONTINUE                                                          YDE 340
C     ------------------------------------------------------------------YDE 350
C         THE DERIVATIVE FOR HEAT CAPACITY OF NON-IONIC SPECIES.        YDE 360
C     ------------------------------------------------------------------YDE 370
      DYDC(1)=ONE                                                       YDE 380
      DYDC(2)=TWO*T                                                     YDE 390
      DYDC(3)=ONE/(T*T)                                                 YDE 400
      DYDC(4)=ZERO                                                      YDE 410
      DYDC(5)=ZERO                                                      YDE 420
      DYDC(6)=T*T                                                       YDE 430
      DYDC(7)=ONE/DSQRT(T)                                              YDE 440
      RETURN                                                            YDE 450
  200 CONTINUE                                                          YDE 460
C     ------------------------------------------------------------------YDE 470
C         THE DERIVATIVE FOR ENTROPY OF NON-IONIC SPECIES.              YDE 480
C     ------------------------------------------------------------------YDE 490
      DYDC(1)=DLOG(T)                                                   YDE 500
      DYDC(2)=TWO*T                                                     YDE 510
      DYDC(3)=-ONE/(TWO*T*T)                                            YDE 520
      DYDC(4)=ZERO                                                      YDE 530
      DYDC(5)=ONE                                                       YDE 540
      DYDC(6)=T*T/TWO                                                   YDE 550
      DYDC(7)=-TWO/DSQRT(T)                                             YDE 560
      RETURN                                                            YDE 570
  300 CONTINUE                                                          YDE 580
C     ------------------------------------------------------------------YDE 590
C         THE DERIVATIVE FOR THE ENTHALPY OF NON-IONIC SPECIES.         YDE 600
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C     ------------------------------------------------------------------YDE 610
      DYDC(1)=T                                                          YDE 620
      DYDC(2)=T*T                                                        YDE 630
      DYDC(3)=-CNE/T                                                     YDE 640
      DYDC(4)=ONE                                                        YDE 650
      DYDC(5)=ZERO                                                       YDE 660
      DYDC(6)=(T**3)/THREE                                               YDE 670
      DYDC(7)=TWO*DSQRT(T)                                               YDE 680
      RETURN                                                             YDE 690
  400 CONTINUE                                                           YDE 700
C     ------------------------------------------------------------------YDE 710
C         THE DERIVATIVE FOR THE GIBBS ENERGY OF NON-IONIC SPECIES.      YDE 720
C     ------------------------------------------------------------------YDE 730
      DYDC(1)=T-T*DLOG(T)                                                YDE 740
      DYDC(2)=-T*T                                                       YDE 750
      DYDC(3)=-CNE/(TWO*T)                                               YDE 760
      DYDC(4)=ONE                                                        YDE 770
      DYDC(5)=-T                                                         YDE 780
      DYDC(6)=-(T**3)/SIX                                                YDE 790
      DYDC(7)=FOUR*DSQRT(T)                                              YDE 800
      RETURN                                                             YDE 810
  500 CONTINUE                                                           YDE 820
C     ------------------------------------------------------------------YDE 830
C         THE DERIVATIVE FOR THE EQUILIBRIUM CONSTANT OF ION-IONIC       YDE 840
C             SPECIES.                                                   YDE 850
C     ------------------------------------------------------------------YDE 860
      DYDC(1)=(DLOG(T)-CNE)/R                                            YDE 870
      DYDC(2)=T/R                                                        YDE 880
      DYDC(3)=ONE/(TWO*R*T*T)                                            YDE 890
      DYDC(4)=-CNE/(R*T)                                                 YDE 900
      DYDC(5)=ONE/R                                                      YDE 910
      DYDC(6)=(T*T)/(SIX*R)                                              YDE 920
      DYDC(7)=-FOUR/(R*DSQRT(T))                                         YDE 930
      RETURN                                                             YDE 940
  600 CONTINUE                                                           YDE 950
C     ------------------------------------------------------------------YDE 960
C         THE DERIVATIVE FOR THE CELL POTENTIAL FOR NON-IONIC SPECIES.   YDE 970
C     ------------------------------------------------------------------YDE 980
      DYDC(1)=(T*DLOG(T)-T)/F                                            YDE 990
      DYDC(2)=(T*T)/F                                                    YDE1000
      DYDC(3)=ONE/(TWO*F*T)                                              YDE1010
      DYDC(4)=-ONE/F                                                     YDE1020
      DYDC(5)=T/F                                                        YDE1030
      DYDC(6)=(T**3)/(SIX*F)                                             YDE1040
      DYDC(7)=-FOUR*DSQRT(T)/F                                           YDE1050
      RETURN                                                             YDE1060
  700 CONTINUE                                                           YDE1070
C     ------------------------------------------------------------------YDE1080
C         THE DERIVATIVE FOR THE RELATIVE HEAT CONTENT OF NON-IONIC      YDE1090
C             SPECIES.                                                   YDE1100
C     ------------------------------------------------------------------YDE1110
      IF (SC.LT.0) GO TO 800                                             YDE1120
      DYDC(1)=T                                                          YDE1130
      DYDC(2)=T*T                                                        YDE1140
      DYDC(3)=-CNE/T                                                     YDE1150
      DYDC(4)=ONE                                                        YDE1160
      DYDC(5)=ZERO                                                       YDE1170
      DYDC(6)=(T**3)/THREE                                               YDE1180
      DYDC(7)=TWO*DSQRT(T)                                               YDE1190
      RETURN                                                             YDE1200
  800 CONTINUE                                                           YDE1210
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      DYCC(1)=TC                                                        YDE1220
      DYCC(2)=TC*TC                                                     YDE1230
      DYCC(3)=-ONE/TC                                                   YDE1240
      DYCC(4)=ONE                                                       YDE1250
      DYCC(5)=ZERO                                                      YDE1260
      DYCC(6)=(TC**3)/THREE                                             YDE1270
      DYCC(7)=TWO*DSQRT(TC)                                             YDE1280
      RETURN                                                            YDE1290
  900 CONTINUE                                                          YDE1300
C     ------------------------------------------------------------------YDE1310
C         THE DERIVATIVE FOR THE HEAT CAPACITY OF IONIC SPECIES.        YDE1320
C     ------------------------------------------------------------------YDE1330
      DYCC(1)=ONE                                                       YDE1340
      DYCC(2)=TWO*T                                                     YDE1350
      DYCC(3)=ONE/(T*T)                                                 YDE1360
      DYCC(4)=ZERO                                                      YDE1370
      DYCC(5)=ZERO                                                      YDE1380
      DYCC(6)=T*T                                                       YDE1390
      ENT=EN(T)                                                         YDE1400
      DYCC(7)=-T*DIE(T)*(A*ENT*A*ENT+A*ENT*A+A*ENT*TWO/THETA+ONE/(THETA*YDE1410
     1THETA))                                                           YDE1420
      RETURN                                                            YDE1430
 1000 CONTINUE                                                          YDE1440
C     ------------------------------------------------------------------YDE1450
C         THE DERIVATIVE FOR THE ENTROPY OF IONIC SPECIES.              YDE1460
C     ------------------------------------------------------------------YDE1470
      DYCC(1)=DLOG(T)                                                   YDE1480
      DYCC(2)=TWO*T                                                     YDE1490
      DYCC(3)=-ONE/(TWO*T*T)                                            YDE1500
      DYCC(4)=ZERO                                                      YDE1510
      DYCC(5)=ONE                                                       YDE1520
      DYCC(6)=T*T/TWO                                                   YDE1530
      DYCC(7)=-DIE(T)*(A*EN(T)+ONE/THETA)                               YDE1540
      RETURN                                                            YDE1550
 1100 CONTINUE                                                          YDE1560
C     ------------------------------------------------------------------YDE1570
C         THE DERIVATIVE FOR THE ENTHALPY OF IONIC SPECIES.             YDE1580
C     ------------------------------------------------------------------YDE1590
      DYCC(1)=T                                                         YDE1600
      DYCC(2)=T*T                                                       YDE1610
      DYCC(3)=-ONE/T                                                    YDE1620
      DYCC(4)=ONE                                                       YDE1630
      DYCC(5)=ZERO                                                      YDE1640
      DYCC(6)=(T**3)/THREE                                              YDE1650
      DYCC(7)=DIE(T)*(ONE-A*T*EN(T)-T/THETA)                            YDE1660
      RETURN                                                            YDE1670
 1200 CONTINUE                                                          YDE1680
C     ------------------------------------------------------------------YDE1690
C         THE DERIVATIVE FOR THE GIBBS ENERGY OF IONIC SPECIES.         YDE1700
C     ------------------------------------------------------------------YDE1710
      DYCC(1)=T-T*DLOG(T)                                               YDE1720
      DYCC(2)=-T*T                                                      YDE1730
      DYCC(3)=-ONE/(TWO*T)                                              YDE1740
      DYCC(4)=ONE                                                       YDE1750
      DYCC(5)=-T                                                        YDE1760
      DYCC(6)=-(T**3)/SIX                                               YDE1770
      DYCC(7)=DIE(T)                                                    YDE1780
      RETURN                                                            YDE1790
 1300 CONTINUE                                                          YDE1800
C     ------------------------------------------------------------------YDE1810
C         THE DERIVATIVE FOR THE EQUILIBRIUM CONSTANT OF IONIC          YDE1820
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C              SPECIES.                                                  YDE1830
C      ----------------------------------------------------------------YDE1840
       DYDC(1)=(DLOG(T)-CNE)/R                                          YDE1850
       DYDC(2)=T/R                                                      YDE1860
       DYDC(3)=CNE/(TWO*R**T*T)                                         YDE1870
       DYDC(4)=-CNE/(R*T)                                               YDE1880
       DYDC(5)=CNE/R                                                    YDE1890
       DYDC(6)=(T*T)/(SIX*R)                                            YDE1900
       DYDC(7)=-DIE(T)/(R*T)                                            YDE1910
       RETURN                                                           YDE1920
  1400 CONTINUE                                                         YDE1930
C      ----------------------------------------------------------------YDE1940
C          THE DERIVATIVE FOR THE CELL POTENTIAL OF IONIC SPECIES.      YDE1950
C      ----------------------------------------------------------------YDE1960
       DYDC(1)=(T*DLOG(T)-T)/F                                          YDE1970
       DYDC(2)=(T*T)/F                                                  YDE1980
       DYDC(3)=CNE/(TWO*F*T)                                            YDE1990
       DYDC(4)=-CNE/F                                                   YDE2000
       DYDC(5)=T/F                                                      YDE2010
       DYDC(6)=(T**3)/(SIX*F)                                           YDE2020
       DYDC(7)=-DIE(T)/F                                                YDE2030
       RETURN                                                           YDE2040
  1500 CONTINUE                                                         YDE2050
C      ----------------------------------------------------------------YDE2060
C          THE DERIVATIVE FOR THE RELATIVE HEAT CONTENT OF IONIC        YDE2070
C              SPECIES.                                                 YDE2080
C      ----------------------------------------------------------------YDE2090
       IF (SC.LT.0) GO TO 1600                                          YDE2100
       DYDC(1)=T                                                        YDE2110
       DYDC(2)=T*T                                                      YDE2120
       DYDC(3)=-CNE/T                                                   YDE2130
       DYDC(4)=ONE                                                      YDE2140
       DYDC(5)=ZERO                                                     YDE2150
       DYDC(6)=(T**3)/THREE                                             YDE2160
       DYDC(7)=DIE(T)*(CNE-A*T*FN(T)-T/THETA)                           YDE2170
       RETURN                                                           YDE2180
  1600 CONTINUE                                                         YDE2190
       DYDC(1)=TC                                                       YDE2200
       DYDC(2)=TC*TC                                                    YDE2210
       DYDC(3)=-CNE/TC                                                  YDE2220
       DYDC(4)=ONE                                                      YDE2230
       DYDC(5)=ZERO                                                     YDE2240
       DYDC(6)=(TC**3)/THREE                                            YDE2250
       DYDC(7)=DIE(TC)*(CNE-A*TC*FN(TC)-TC/THETA)                       YDE2260
       RETURN                                                           YDE2270
C      ----------------------------------------------------------------YDE2280
       END                                                              YDE2290-
```

```
      SUBROUTINE DDERIV (T)                                                 DDE  10
C     ------------------------------------------------------------------DDF  20
C                                                                         DDE  30
C                                  DDERIV                                 DDE  40
C                                                                         DDE  50
C     THIS VERSION WAS WRITEN 3/09/72 BY HAAS.                            DDF  60
C          LAST REVISED 8/05/72 BY HAAS.                                  DDE  70
C                                                                         DDE  80
C     ------------------------------------------------------------------DDF  90
      IMPLICIT REAL*8(A-H,O-Z)                                            DDD 100
      DIMENSION DDDC(7),SCINV(2),DYCC(7)                                  DDE 110
C     ------------------------------------------------------------------DDE 120
C          COMMON BLOCKS                                                  DDE 130
C             NAME              ROUTINES                                  DDE 140
C               EARTH             MAIN PROGRAM, DRGLS2, EAFW20, PLTOUT    DDE 150
C               AIR               MAIN PROGRAM, DRGLS2, TEST20, EAFW20    DDE 160
C                                 PUTOUT AND UNIQUE.                      DDE 170
C               FIRE              MAIN PROGRAM, DRGLS2, TEST20, EAFW20    DDE 180
C               WATER             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,   DDE 190
C                                 PUTOUT, FN, CIE, AND PLOCK DATA.        DDE 200
C               TIME              MAIN PROGRAM, PLTOUT                    DDE 210
C               SPACE             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,   DDE 220
C                                    AND PUTPLT                           DDE 230
C               MAN               MAIN PROGRAM, PLTOUT                    DDE 240
C     ------------------------------------------------------------------DDE 250
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, P,               DDE 260
     1  SCINV, TREF, STDDEF, DIEO, A, B, THETA                            DDF 270
      COMMON /SPACE/ DDDC, DYCC, SC, TC                                   DDE 280
C     ------------------------------------------------------------------DDE 290
C     CALCULATE THE DERIVATIVE OF -D- WITH RESPECT TO THE OTHER           DDE 300
C          CONSTANTS WHERE THE GIBBS ENERGY IS 0.0 AS IS THE              DDE 310
C          CASE FOR ELEMENTS AT 298.15 KELVIN OR AT THE TEMPERATURE OF    DDE 320
C          INVERSION.                                                     DDE 330
C     ------------------------------------------------------------------DDE 340
      DDDC(1)=T*DLOG(T)-T                                                 DDE 350
      DDDC(2)=T*T                                                         DDE 360
      DDDC(3)=ONE/(TWO*T)                                                 DDE 370
      DDDC(4)=-ONE                                                        DDE 380
      DDDC(5)=T                                                           DDE 390
      DDDC(6)=(T**3)/SIX                                                  DDE 400
      DDDC(7)=-FOUR*DSQRT(T)                                              DDE 410
      RETURN                                                              DDE 420
      END
```

```
      DOUBLE PRECISION FUNCTION DIE(T)                                  DIE  10
      IMPLICIT REAL*8(A-H,O-Z)                                          DIE  20
      DIMENSION STCOEF(10),SCINV(2)                                     DIE  30
C     ------------------------------------------------------------------DIE  40
C         COMMON BLOCKS                                                 DIE  50
C            NAME             ROUTINES                                 DIE  60
C              EARTH            MAIN PROGRAM, ORGLS2, EAFW20, PUTOUT   DIE  70
C              AIR              MAIN PROGRAM, ORGLS2, TEST20, EAFW20   DIE  80
C                               PUTOUT AND UNIGLE.                     DIE  90
C              FIRE             MAIN PROGRAM, ORGLS2, TEST20, EAFW20   DIE 100
C              WATER            MAIN PROGRAM, EAFW20, YDERIV, DDERIV,  DIE 110
C                               PUTOUT, FN, DIS, AND BLOCK DATA.       DIE 120
C              TIME             MAIN PROGRAM, PUTOUT                   DIE 130
C              SPACE            MAIN PROGRAM, EAF420, YDERIV, DDERIV,  DIE 140
C                                  AND PUTPUT                          DIE 150
C              MAN              MAIN PROGRAM, PUTOUT                   DIE 160
C     ------------------------------------------------------------------DIE 170
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, H, E,             DIE 180
     1  SCINV, TRUE, STCOEF,DI20,A,B,THETA                              DIE 190
      DIE=DEXP(FN(T)*T/THETA)/DI20                                      DIE 200
      RETURN                                                            DIE 210
      END                                                               DIE 220-
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      DOUBLE PRECISION FUNCTION FN(T)                                    FN   10
      IMPLICIT REAL*8(A-H,O-Z)                                           FN   20
      DIMENSION STCOEF(10),SCINV(2)                                      FN   30
C     ------------------------------------------------------------------FN   40
C                                                                        FN   50
C         COMMON BLOCKS                                                  FN   60
C            NAME              ROUTINES                                  FN   70
C              EARTH             MAIN PROGRAM, ORCLS2, EAFW20, PUTOUT    FN   80
C              AIR               MAIN PROGRAM, ORCLS2, TEST2D, EAFW20    FN   90
C                                PUTOUT AND UNIQUE.                      FN  100
C              FIRE              MAIN PROGRAM, ORCLS2, TEST2D, EAFW20    FN  110
C              WATER             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,   FN  120
C                                PUTOUT, FN, DIE, AND BLOCK DATA.        FN  130
C              TIME              MAIN PROGRAM, PLTOUT                    FN  140
C              SPACE             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,   FN  150
C                                   AND PUTPUT                           FN  160
C              MAN               MAIN PROGRAM, PLTOUT                    FN  170
C     ------------------------------------------------------------------FN  180
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,              FN  190
     1  SCINV, TREF, STCOEF,DIFO,A,B,THETA                               FN  200
      FN=DEXP(B*A*T)                                                     FN  210
      RETURN                                                             FN  220
      END
```

```
      SUBROUTINE UNIQUE (YC,I,J,JDFLAG)                                 UNI  10
C     ------------------------------------------------------------------UNI  20
C     DUMMY SUBROUTINE UNIQUE  --  RETURNS ERROR STATEMENT IF CALLED.   UNI  30
C                                                                       UNI  40
C     UNIQUE IS TO BE PROGRAMMED BY THE USER.  UNIQUE IS INTENDED       UNI  50
C         TO SUPPLY YC AND  DC(KI(NP).NE.0)  FOR THOSE DATA SETS NOT    UNI  60
C         COVERED BY THE ROUTINES EAFW20, YDERIV, AND DDERIV.           UNI  70
C                                                                       UNI  80
C     THE SUBROUTINE UNIQUE WILL BE CALLED WHEN THE INDEX IGO(J) IS     UNI  90
C         GREATER THAN 7.                                               UNI 100
C                                                                       UNI 110
C             ARGUMENTS--                                               UNI 120
C                  YC -- YCALC RETURNED BY UNIQUE FROM CURRENT VALUES OFUNI 130
C                        THE PARAMETERS P(I).                           UNI 140
C                  I -- INDEX FOR THE I-TH OBSERVATION.                 UNI 150
C                  J -- INDEX FOR THE J-TH DATA SET.                    UNI 160
C                  JDFLAG -- IF UNIQUE IS CALLED AT REGRESSION TIME,    UNI 170
C                              JDFLAG IS ZERO AND THE DERIVATIVES       UNI 180
C                              DC(I) MUST BE RETURNED.                  UNI 190
C                            IF UNIQUE IS CALLED AT PLOT TIME, JDFLAG   UNI 200
C                              IS NOT ZERO AND THE DERIVATIVES NEED     UNI 210
C                              NOT BE RETURNED.                         UNI 220
C     ------------------------------------------------------------------UNI 230
      IMPLICIT REAL*8(A-H,O-Z)                                          UNI 240
      DIMENSION COEF(6,70),FNAME(20),TINV(6,70,4),IPHASE(5,70),         UNI 250
     1  NPHASE(70),IKOUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),        UNI 260
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                          UNI 270
C     ------------------------------------------------------------------UNI 280
C        COMMON BLOCKS                                                  UNI 290
C           NAME              ROUTINES                                  UNI 300
C             EARTH             MAIN PROGRAM, CRGLS2, EAFW20, PUTOUT    UNI 310
C             AIR               MAIN PROGRAM, CRGLS2, TEST20, EAFW20    UNI 320
C                               PUTOUT AND UNIGLE.                      UNI 330
C             FIRE              MAIN PROGRAM, CRGLS2, TEST20, EAFW20    UNI 340
C             WATER             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,   UNI 350
C                               PUTOUT, FN, DIF, AND PLOCK DATA.        UNI 360
C             TIME              MAIN PROGRAM, PLTOUT                    UNI 370
C             SPACE             MAIN PROGRAM, EAFW20, YDERIV, DDERIV,   UNI 380
C                                 AND PUTPUT                            UNI 390
C             MAN               MAIN PROGRAM, PLTCLT                    UNI 400
C     ------------------------------------------------------------------UNI 410
      COMMON /EARTH/ COEF,FNAME,TINV,IPHASE,NPHASE,IKOUNT,IGO,NSETS,    UNI 420
     1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                          UNI 430
      WRITE (6,100) J,J,IGO(J)                                          UNI 440
      STOP                                                              UNI 450
  100 FORMAT (6H0YOUR ,I3,35H-TH DATA SET CALLED UNIQUE FROM EAFW20./5H UNI 460
     1IGO(,I2,17H) HAS A VALUE OF ,I6,38H BUT UNIQUE IS CURRENTLY UNPROGUNI 470
     2RAMMED.)                                                          UNI 480
      END                                                               UNI 490-
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      SUBROUTINE PLTOUT (J)                                                 PUT  10
      IMPLICIT REAL*8(A-H,O-Z)                                              PUT  20
      LOGICAL*1 BCC,LABEL                                                   PUT  30
      REAL*4 TITLE,ACCFF                                                    PLT  40
      DIMENSION SGN(2),A(7,7)                                               PUT  50
      DIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),             PUT  60
     1  NPHASE(70),IKOUNT(70),IGO(70),ISTATE(6,70),NINVER(6,70),            PUT  70
     2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)                              PUT  80
      DIMENSION X(2,1200),YO(1200),SIGYO(1200),P(140),KI(140),              PLT  90
     1  DO(140),PD(140),TITLE(20)                                           PUT 100
      DIMENSION SCINV(2),STCOEF(10),YESNO(2),TK(19,2),TYPE(14),NSCALE(5)PUT 110
     1  ,LABEL(50)                                                          PUT 120
      DIMENSION DDOO(7),DYDO(7)                                           PUT 130
      DIMENSION AA (140)                                                  PUT 140
C     ------------------------------------------------------------------PUT 150
C         COMMON BLOCKS                                                   PLT 160
C            NAME              ROUTINES                                   PLT 170
C              EARTH             MAIN PROGRAM, ORGLS2, SAFW20, PUTOUT     PUT 180
C              AIR               MAIN PROGRAM, ORGLS2, TEST20, SAFW20     PUT 190
C                                PUTOUT AND UNIQUE.                       PUT 200
C              FIRE              MAIN PROGRAM, ORGLS2, TEST20, SAFW20     PUT 210
C              WATER             MAIN PROGRAM, SAFW20, YDERIV, DDERIV,    PUT 220
C                                PUTOUT, FN, DIE, AND PLOCK DATA.         PUT 230
C              TIME              MAIN PROGRAM, PLTOUT                     PUT 240
C              SPACE             MAIN PROGRAM, SAFW20, YDERIV, DDERIV,    PLT 250
C                                   AND PLTPLT                            PUT 260
C              MAN               MAIN PROGRAM, PLTOUT                     PUT 270
C     ------------------------------------------------------------------PUT 280
      COMMON /EARTH/ COEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGO,NSETS,      PUT 290
     1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP                              PUT 300
      COMMON /AIR/ X, P, DO, TITLE, YO, SIGYO, PD, KI, NO, NV, NX, IW,    PUT 310
     1  NP, ND, ISING, ISTOP, IL, JDFLAG                                    PUT 320
      COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, E, F,               PLT 330
     1  SCINV, TREF, STCOEF, DIEO, ADIS, BDIE, THETA, YESNO, TK,            PLT 340
     2  ASTAR, TYPE, NL, NSCALE, LABEL, BCC                                 PUT 350
      COMMON /TIME/ DATE                                                  PUT 360
      COMMON /SPACE/ DDOO, DYDO, SC, TO                                   PUT 370
      COMMON /MAN/ AA                                                     PLT 380
      CPRIME=ZERO                                                         PUT 390
      LSTPHA=NPHASE(J)                                                    PUT 400
      DO 1200 L=1,LSTPHA                                                  PUT 410
      INDEX=1+(IPHASE(L,J)-1)                                             PUT 420
      D=0.000                                                             PUT 430
      IF (ISTATE(L,J).NE.1) GO TO 200                                     PUT 440
      CALL DDERIV (TREF)                                                  PUT 450
      DO 100 K=1,7                                                        PUT 460
      D=D+P(INDEX+K-1)*DDOO(K)                                            PUT 470
  100 CONTINUE                                                            PUT 480
      GO TO 900                                                           PUT 490
  200 CONTINUE                                                            PUT 500
      IF (NINVER(L,J).EQ.0) GO TO 900                                     PUT 510
      DO 300 I=1,2                                                        PUT 520
      SGN(I)=SCINV(I)                                                     PUT 530
  300 CONTINUE                                                            PUT 540
      IF (INVSC(L,J).EQ.0) GO TO 500                                      PUT 550
      DO 400 LLL=1,2                                                      PUT 560
      SGN(LLL)=SGN(LLL)*STCOEF(INVSC(L,J))                                PUT 570
  400 CONTINUE                                                            PUT 580
  500 CONTINUE                                                            PUT 590
      IF (INSTAT(L,J).EQ.0) GO TO 700                                     PUT 600
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      INDEX2=I+7*(INVPH(L,J,1)-1)                                       PUT 610
      CALL DDERIV (TREF)                                                PUT 620
      DO 600 K=I,7                                                      PUT 630
      D=D+P(INDEX2+K-I)*DCOC(K)*SGN(2)                                  PUT 640
  600 CONTINUE                                                          PUT 650
  700 CONTINUE                                                          PUT 660
      LSTINV=NINVER(L,J)                                                PUT 670
      DO 800 LST=1,LSTINV                                               PUT 680
      IF ((LST.EQ.LSTINV).AND.(INVSC(L,J).NE.0)) SGN(2)=SGN(2)/STCOEF(INPUT 690
     1VSC(L,J))                                                         PUT 700
      CALL DDERIV (TINV(L,J,LST))                                       PUT 710
      DO 800 LLL=1,2                                                    PUT 720
      INDEX2=1+7*(INVPH(L,J,LST+LLL-1)-1)                               PUT 730
      DO 800 K=I,7                                                      PUT 740
      D=D+P(INDEX2+K-I)*DCOC(K)*SGN(LLL)                                PUT 750
  800 CONTINUE                                                          PUT 760
  900 CONTINUE                                                          PUT 770
      DO 1000 K=I,7                                                     PUT 780
      A(L,K)=P(INDEX+K-1)                                               PUT 790
 1000 CONTINUE                                                          PUT 800
      A(L,4)=A(L,4)+D                                                   PUT 810
      DO 1100 K=I,7                                                     PUT 820
      AA(INDEX+K-1)=A(L,K)                                              PUT 830
 1100 CONTINUE                                                          PUT 840
 1200 CONTINUE                                                          PUT 850
      LST=LSTPHA+1                                                      PUT 860
      DO 1300 K=1,7                                                     PUT 870
      A(LST,K)=0.000                                                    PUT 880
 1300 CONTINUE                                                          PUT 890
      DO 1500 L=I,LSTPHA                                                PUT 900
      DO 1500 K=I,7                                                     PUT 910
      IF ((K.EQ.7).AND.(ISTATE(L,J).EQ.-1)) GO TO 1400                  PUT 920
      A(LST,K)=A(LST,K)+A(L,K)*COEF(L,J)                                PUT 930
      GO TO 1500                                                        PUT 940
 1400 CPRIME=CPRIME+A(L,K)*COEF(L,J)                                    PUT 950
 1500 CONTINUE                                                          PUT 960
      WRITE (6,1900) DATE                                               PUT 970
      DO 1600 L=I,LSTPHA                                                PUT 980
      ACOEF=COEF(L,J)                                                   PUT 990
      WRITE (6,2000) PNAME(IPHASE(L,J)),ACOEF,(A(L,K),K=1,7)            PUT1000
 1600 CONTINUE                                                          PUT1010
      IF ((NPHASE(J).EQ.I).OR.(IGO(J).GE.7)) GO TO 1800                 PUT1020
      IF (CPRIME.EQ.ZERO) GO TO 1700                                    PUT1030
      WRITE (6,2200)                                                    PUT1040
      WRITE (6,2300) (A(LST,K),K=1,7),CPRIME                            PUT1050
      GO TO 1800                                                        PUT1060
 1700 CONTINUE                                                          PUT1070
      WRITE (6,2100)                                                    PUT1080
      WRITE (6,2300) (A(LST,K),K=1,7)                                   PUT1090
 1800 CONTINUE                                                          PUT1100
      RETURN                                                            PUT1110
 1900 FORMAT (1HO/1HO,A8,10H----------/6HOPHASE,8X,4HCOEF,9X,7H'A'/'G',1PUT1120
     13X,3H'B',15X,3H'C',15X,3H'D',15X,3H'E',15X,3H'F')                  PUT1130
 2000 FORMAT (1HO,A8,4X,F6.3,1X,1P6D18.7/1H ,19X,1PD18.7)               PUT1140
 2100 FORMAT (1HO/1HO,26X,7H'A'/'G',13X,3H'B',15X,3H'C',15X,3H'D',15X,3HPUT1150
     1'E',15X,3H'F')                                                    PUT1160
 2200 FORMAT (1HO/1HO,26X,7H'A'/'G',9X,12H'B'/'C(ION)',10X,3H'C',15X,3H'PUT1170
     1D',15X,3H'E',15X,3H'F')                                           PUT1180
 2300 FORMAT (20HOREACTION CONSTANTS ,1P6D18.7/(1H ,19X,1P2D18.7))      PUT1190
      END                                                               PUT1200-
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      SUBROUTINE PRPLOT                                                 PRP  10
      IMPLICIT LOGICAL*1(W),LOGICAL*1(K)                                PRP  20
      DIMENSION NSCALE(5), ABNOS(26), X(1), Y(1)                        PRP  30
      LOGICAL*1 NOS(10)/'0','1','2','3','4','5','6','7','8','9'/       PRP  40
      LOGICAL*1 IMAGE(5CC0),CH ,LABEL(50)                               PRP  50
      LOGICAL*1 VC,HC,FOR1(19),FOR2(15),FOR3(19),NC,BL,HF,HF1           PRP  60
      REAL*8 FOX1(3),FOX2(2),FOX3(3)                                    PRP  70
      INTEGER*2 VCR                                                     PRP  80
      EQUIVALENCE(FOR1,FOX1),(FOR2,FOX2),(FOR3,FOX3),(VC,VCR)           PRP  90
      DATA HC/'-'/,NC/'+'/,BL/' '/,HF/'F'/,HF1/'.'/                     PRP 100
      DATA FOX1/'(1XA1,F9',',2,  121','A1)     '/                       PRP 110
      DATA FOX2/'(1XA1, 9','X121A1) '/                                  PRP 120
      DATA FOX3/'(1HOF  .',' ,  F   ','. )     '/                       PRP 130
      DATA VCR/24F00/                                                   PRP 140
      DATA KPLOT1/.FALSE./,KPLOT2/.FALSE./                              PRP 150
      DATA KABSC,KORD,KPCTGL/3*.FALSE./                                 PRP 160
C                                                                       PRP 170
      ENTRY PLOT1(NSCALE,NFL,NSBH,NVL,NSBV)                             PRP 180
      KPLOT1=.TRUE.                                                     PRP 190
      KPLOT2=.FALSE.                                                    PRP 200
      NH=IABS(NFL)                                                      PRP 210
      NSH=IABS(NSBH)                                                    PRP 220
      NV=IABS(NVL)                                                      PRP 230
      NSV=IABS(NSBV)                                                    PRP 240
      NSCL=NSCALE(1)                                                    PRP 250
      IF (NH*NSH*NV*NSV.NE.0) GO TO 200                                 PRP 260
      WRITE (6,100)                                                     PRP 270
  100 FORMAT (T5,'SOME PLOT1 ARG. ILLEGALLY 0')                         PRP 280
      KPLOT=.FALSE.                                                     PRP 290
      RETURN                                                            PRP 300
  200 KPLOT=.TRUE.                                                      PRP 310
      IF (NV.LE.25) GO TO 400                                           PRP 320
      WRITE (6,300)                                                     PRP 330
      KPLOT=.FALSE.                                                     PRP 340
  300 FORMAT (T5,'NO. OF VERTICAL LINES >25')                           PRP 350
      RETURN                                                            PRP 360
  400 CONTINUE                                                          PRP 370
      NVM=NV-1                                                          PRP 380
      NVP=NV+1                                                          PRP 390
      NDH=NH*NSH                                                        PRP 400
      NDHP=NDH+1                                                        PRP 410
      NDV=NV*NSV                                                        PRP 420
      NDVP=NDV+1                                                        PRP 430
      NIMG=(NDHP*NDVP)                                                  PRP 440
      IF (NDV.LE.120) GO TO 600                                         PRP 450
      KPLOT=.FALSE.                                                     PRP 460
      WRITE (6,500)                                                     PRP 470
  500 FORMAT (T5,'WIDTH OF GRAPH >121')                                 PRP 480
      RETURN                                                            PRP 490
  600 CONTINUE                                                          PRP 500
      IF (NSCL.EQ.0) GO TO 700                                          PRP 510
      FSY=10.**NSCALE(2)                                                PRP 520
      FSX=10.**NSCALE(4)                                                PRP 530
      IY=MIN0(IABS(NSCALE(3)),7)+1                                      PRP 540
      IX=MIN0(IABS(NSCALE(5)),9)+1                                      PRP 550
      GO TO 800                                                         PRP 560
  700 FSY=1.                                                            PRP 570
      FSX=1.                                                            PRP 580
      IY=4                                                              PRP 590
      IX=4                                                              PRP 600
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  800 FOR1(10)=NCS(1Y)                                                  PRP 610
      NA=MIN0(I),NSV)-1                                                 PRP 620
      NS=NA-MIN0(NA,120-NOV)                                            PRP 630
      NB=11-NS+NA                                                       PRP 640
      I1=NB/10                                                          PRP 650
      I2=NB-I1*10                                                       PRP 660
      FOR3(6)=NCS(I1+1)                                                 PRP 670
      FOR3(7)=NCS(I2+1)                                                 PRP 680
      FOR3(9)=NCS(NA+1)                                                 PRP 690
      IF (NV.GT.0) GO TO 1000                                           PRP 700
      DO 900 J=11,18                                                    PRP 710
  900 FOR3(J)=BL                                                        PRP 720
      GO TO 1100                                                        PRP 730
 1000 I1=NV/10                                                          PRP 740
      I2=NV-I1*10                                                       PRP 750
      FOR3(11)=NCS(I1+1)                                                PRP 760
      FOR3(12)=NCS(I2+1)                                                PRP 770
      FOR3(13)=PF                                                       PRP 780
      I1=NSV/100                                                        PRP 790
      I3=NSV-I1*100                                                     PRP 800
      I2=I3/10                                                          PRP 810
      I3=I3-I2*10                                                       PRP 820
      FOR3(14)=NOS(I1+1)                                                PRP 830
      FOR3(15)=NCS(I2+1)                                                PRP 840
      FOR3(16)=NCS(I3+1)                                                PRP 850
      FOR3(17)=PF1                                                      PRP 860
      FOR3(18)=FOR3(9)                                                  PRP 870
 1100 IF (KPLOT1) RETURN                                                PRP 880
      KPLOT1=.TRUE.                                                     PRP 890
C                                                                       PRP 900
      ENTRY PLOT2(IMAGE,XMAX,XMIN,YMAX,YMIN)                            PRP 910
      KPLOT2=.TRUE.                                                     PRP 920
      IF (KPLOT1) GO TO 1200                                            PRP 930
      NSCL=0                                                            PRP 940
      NH=5                                                              PRP 950
      NSH=10                                                            PRP 960
      NV=10                                                             PRP 970
      NSV=10                                                            PRP 980
      GO TO 200                                                         PRP 990
 1200 CONTINUE                                                          PRP1000
      IF (.NOT.KPLOT) RETURN                                            PRP1010
      YMX=YMAX                                                          PRP1020
      DH=(YMAX-YMIN)/FLOAT(NDH)                                         PRP1030
      DV=(XMAX-XMIN)/FLOAT(NDV)                                         PRP1040
      DO 1300 I=1,NVP                                                   PRP1050
 1300 ABNOS(I)=(XMIN+FLOAT((I-1)*NSV)*DV)*FSX                           PRP1060
      DO 1400 I=1,NIMG                                                  PRP1070
 1400 IMAGE(I)=BL                                                       PRP1080
      DO 1800 I=1,NOHP                                                  PRP1090
      I2=I*NDVP                                                         PRP1100
      I1=I2-NDV                                                         PRP1110
      KNHOR=MOD(I-1,NSH).NE.0                                           PRP1120
      IF (KNHOR) GO TO 1600                                             PRP1130
      DO 1500 J=11,12                                                   PRP1140
 1500 IMAGE(J)=PC                                                       PRP1150
 1600 CONTINUE                                                          PRP1160
      DO 1800 J=I1,12,NSV                                               PRP1170
      IF (KNHOR) GO TO 1700                                             PRP1180
      IMAGE(J)=AC                                                       PRP1190
      GO TO 1800                                                        PRP1200
 1700 IMAGE(J)=VC                                                       PRP1210
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 1800 CONTINUE                                                          PRP1220
      XMIN1=XMIN-DV/2.                                                  PRP1230
      YMIN1=YMIN-DH/2.                                                  PRP1240
      RETURN                                                            PRP1250
C                                                                       PRP1260
      ENTRY PLOT3(CH,X,Y,N3)                                            PRP1270
      IF (KPLOT2) GO TO 2100                                            PRP1280
 1900 WRITE (6,2000)                                                    PRP1290
 2000 FORMAT (T5,'PLOT2 MUST BE CALLED')                                PRP1300
 2100 CONTINUE                                                          PRP1310
      IF (.NOT.KPLOT) RETURN                                            PRP1320
      IF (N3.GT.0) GO TO 2300                                           PRP1330
      KPLOT=.FALSE.                                                     PRP1340
      WRITE (6,2200)                                                    PRP1350
 2200 FORMAT (T5,'PLOT3, APG2 ) 0')                                     PRP1360
      RETURN                                                            PRP1370
 2300 DO 3000 I=1,N3                                                    PRP1380
      IF (DV) 2500,2400,2500                                            PRP1390
 2400 DUM1=0                                                            PRP1400
      GO TO 2600                                                        PRP1410
 2500 CONTINUE                                                          PRP1420
      DUM1=(X(I)-XMIN1)/DV                                              PRP1430
 2600 IF (DH) 2800,2700,2800                                            PRP1440
 2700 DUM2=0                                                            PRP1450
      GO TO 2900                                                        PRP1460
 2800 CONTINUE                                                          PRP1470
      DUM2=(Y(I)-YMIN1)/DH                                              PRP1480
 2900 CONTINUE                                                          PRP1490
      IF (DUM1.LT.0..OR.DUM2.LT.0.) GO TO 3000                          PPP1500
      IF (DUM1.GE.NDVP.OR.DUM2.GE.NDHP) GO TO 3000                      PPP1510
      NX=1+INT(DUM1)                                                    PPP1520
      NY=1+INT(DUM2)                                                    PRP1530
      J=(NDHP-NY)*NDVP+NX                                               PRP1540
      IMAGE(J)=CH                                                       PPP1550
 3000 CONTINUE                                                          PRP1560
      RETURN                                                            PRP1570
C                                                                       PRP1580
      ENTRY PLOT4(NL,LABEL)                                             PRP1590
      ENTRY EPLOT4(NL,LABEL)                                            PRP1600
      IF (.NOT.KPLOT) RETURN                                            PRP1610
      IF (.NOT.KPLOT2) GO TO 1900                                       PRP1620
      DO 3200 I=1,NDHP                                                  PRP1630
      IF (I.EQ.NDHP.AND.KBOTGL) GO TO 3200                              PRP1640
      WL=BL                                                             PPP1650
      IF (I.LE.NL) WL=LABEL(I)                                          PRP1660
      I2=I*NDVP                                                         PRP1670
      I1=I2-NDV                                                         PRP1680
      IF (MOD(I-1,NSH).EQ.0.AND..NOT.KCRD) GO TO 3100                   PRP1690
      WRITE (6,FOR2) WL,(IMAGE(J),J=I1,I2)                              PRP1700
      GO TO 3200                                                        PPP1710
 3100 CONTINUE                                                          PRP1720
      CRDNO=(YMX-FLOAT(I-1)*DH)*FSY                                     PPP1730
      IF (I.EQ.NDHP) CRDNO=YMIN                                         PRP1740
      WRITE (6,FOR1) WL,CRDNO,(IMAGE(J),J=I1,I2)                        PRP1750
 3200 CONTINUE                                                          PPP1760
      IF (KABSC) GO TO 3300                                             PRP1770
      WRITE (6,FOR3) (ABSCS(J),J=1,NVP)                                 PRP1780
 3300 RETURN                                                            PRP1790
C                                                                       PRP1800
      ENTRY OMIT(LSW)                                                   PRP1810
      KABSC=MOD(LSW,2).EQ.1                                             PRP1820
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KCRD=MJD(LSW,4).GE.2                                    PRP1830
KBCTGL=LSW.GE.4                                         PRP1840
RETURN                                                  PRP1850
END                                                     PRP1860-
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